U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-264 445

Preliminary Scoring of Selected Organic Air Pollutants. Appendix III. Chemistry Production & Toxicity of Chemicals F - N

MITRE Corp, McLean, Va METREK Div

Prepared for

Environmental Protection Agency, Research Triangle Park, N C Office of Air Quality Planning and Standards

Oct 76

PB 264 445

EPA-450/3-77-008d
October 1976

PRELIMINARY SCORING OF SELECTED ORGANIC AIR POLLUTANTS

APPENDIX III - CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS F THROUGH N

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U. S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-450/3-77-008d	2.	3. RECIPIENT'S ACCESSION NO.
4. TITLE AND SUBTITLE Preliminary Scoring of Organic Air Pollutants: Chemistry, Production and Toxicity of Selected Synthetic Organic Chemicals (Chemicals F-N) Appendix III		5. REPORT DATE October 1976
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) J. Dorigan, B. Fuller, R. Duffy		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS The Mitre Corporation Metrek Division Westgate Research Park McLean, Virginia 22101		10. PROGRAM ELEMENT NO.
		11. CONTRACT/GRANT NO. 68-02-1495
12. SPONSORING AGENCY NAME AND ADDRESS EPA, Office of Air Quality Planning and Standards Strategies and Air Standards Division Research Triangle Park, N.C. 27711		13. TYPE OF REPORT AND PERIOD COVERED
		14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES

16. ABSTRACT

This is the third of a series of four appendices to the report "Scoring of Organic Air Pollutants." The entire appendix contains a compilation of available data on chemical structure and properties, environmental persistence, production, and toxicity for 637 synthetic organic chemicals. This third volume covers the chemicals ferbam through nonyl phenol.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
organic chemical structure organic chemical properties organic chemical production organic chemical toxicity		

18. DISTRIBUTION STATEMENT unlimited	19. SECURITY CLASS *(This Report)* unclassified	21. NO. OF PAGES 312
	20. SECURITY CLASS *(This page)* unclassified	22. PRICE

EPA Form 2220-1 (9-73)

EPA-450/3-77-008d

PRELIMINARY SCORING OF SELECTED ORGANIC AIR POLLUTANTS APPENDIX III - CHEMISTRY, PRODUCTION, AND TOXICITY OF CHEMICALS F THROUGH N

by

J. Dorigan, B. Fuller and R. Duffy

The Mitre Corporation
Metrek Division
Westgate Research Park
McLean, Virginia 22101

Contract No. 68-02-1495

Project No. 077L

EPA Project Officer: David R. Patrick

Prepared for

ENVIRONMENTAL PROTECTION AGENCY
Office of Air and Waste Management
Office of Air Quality Planning and Standards
Research Triangle Park, North Carolina 27711

October 1976

i (a)

PREFACE

A program is being developed by the Emission Standards and Engineering Division of the U.S. Environmental Protection Agency to determine the extent and environmental effects of atmospheric industrial emissions of synthetic organic chemicals. As part of the initial effort, EPA requested that the MITRE Corporation, METREK Division, devise a system for identifying those chemicals that may be released to the atmosphere from chemical manufacturing plants and whose health effects have been documented. To address this need, three general categories of information for each compound to be evaluated were deemed directly relevant:

(1) the quantity of the compound produced;

(2) the potential for atmospheric release from chemical manufacturing plants, and

(3) the toxicological effects of the compounds.

The results of this study are presented in the accompanying report "Preliminary Scoring of Organic Air Pollutants."

The following dossiers were prepared for each of the 637 compounds under consideration in an attempt to collate the pertinent data for subsequent evaluation.

TABLE OF CONTENTS

	Page
Ferbam	AIII-2
Ferrocene	AIII-4
Fluometuron	AIII-6
Folex	AIII-8
Folpet	AIII-10
Formaldehyde	AIII-12
Formamide	AIII-14
Formic acid	AIII-16
Fumaric acid	AIII-18
Furfural	AIII-20
Furfuryl alcohol	AIII-22
Glycerol	AIII-24
Glycerol monostearate	AIII-26
Glycidol	AIII-28
Glycine	AIII-30
Glyoxal	AIII-32
Guanidine	AIII-34
Guthion	AIII-36
Heptachlor	AIII-38
Heptene	AIII-40
Herban	AIII-42
Hexachloroethane	AIII-44
Hexachloronaphthalene	AIII-46
Hexalene glycol	AIII-48
Hexamethylenetetramine	AIII-50
Hexanediamine	AIII-52
Hydrogen cyanide	AIII-54
Hydroquinone	AIII-56
Indene	AIII-58
Isoamyl alcohol	AIII-60
Isobutyl acetate	AIII-62
Isobutyl alcohol	AIII-64
Isobutylaldehyde	AIII-66
Isobutylene	AIII-68
Isobutyric acid	AIII-70
Isodecyl alcohol	AIII-72
Isooctyl alcohol	AIII-74
Isooctylphenol, ethoxylated	AIII-76
Isophorone	AIII-78
Isophthalic acid	AIII-80
Isoprene	AIII-82
Isopropyl acetate	AIII-84
Isopropyl alcohol	AIII-86
Isopropylamine	AIII-88

TABLE OF CONTENTS (Continued)

	Page
Isopropyl chloride	AIII-90
Isopropyl ether	AIII-92
o-Isopropylphenol	AIII-94
p-Isopropylphenol	AIII-96
Ketene	AIII-98
Ligninsulfonic acid, ammonium salt	AIII-100
Ligninsulfonic acid, calcium salt	AIII-102
Ligninsulfonic acid, ferrochrome salt	AIII-104
Ligninsulfonic acid, sodium salt	AIII-106
Lindane	AIII-108
Linuron	AIII-110
Magenta	AIII-112
Malathion	AIII-114
Maleic acid	AIII-116
Maleic anhydride	AIII-118
Maleic hydrazide	AIII-120
Malic acid	AIII-122
Melamine	AIII-124
Mesitylene	AIII-126
Mesityl oxide	AIII-128
Methacrylic acid	AIII-130
Methacrylonitrile	AIII-132
Methallyl alcohol	AIII-134
Methallyl chloride	AIII-136
Methane	AIII-138
Methanearsonic acid	AIII-140
Methomyl	AIII-142
Methoxychlor	AIII-144
Methoxyethanol	AIII-146
Methyl acetate	AIII-148
Methyl acetoacetate	AIII-150
Methylal	AIII-152
Methyl alcohol	AIII-154
Methylamine	AIII-156
Methylamyl acetate	AIII-158
Methylamyl alcohol	AIII-160
Methylaniline	AIII-162
Methylbenzyl alcohol	AIII-164
Methyl bromide	AIII-166
Methyl butyl ketone	AIII-168
Methylbutynol	AIII-170
Methyl cellulose	AIII-172
Methyl chloride	AIII-174
Methylcholanthrene	AIII-176

TABLE OF CONTENTS (Continued)

	Page
Methylcyclohexane	AIII-178
Methylcyclohexanol	AIII-180
Methylcyclohexanone	AIII-182
4,4'-Methylenebis (2-chloroaniline)	AIII-184
Methylene chloride	AIII-186
Methylenedianiline	AIII-188
Methyldioxolane	AIII-190
Methyl ethyl ketone	AIII-192
Methyl formate	AIII-194
Methylhydrazine	AIII-196
Methyl iodide	AIII-198
Methyl isoamyl ketone	AIII-200
Methyl isobutyl ketone	AIII-202
Methyl isocyanate	AIII-204
Methyl mercaptan	AIII-206
Methyl methacrylate	AIII-208
Methylnaphthalene	AIII-210
N-Methyl-N'-nitro-N-nitrosoguaindine	AIII-212
Methyl parathion	AIII-214
Methylpentanediol	AIII-216
Methylpentynol	AIII-218
Methylphenylcarbinol	AIII-220
α-Methylstyrene	AIII-222
Mevinphos	AIII-224
Mirex	AIII-226
Monosodium glutamate	AIII-228
Morpholine	AIII-230
MSMA	AIII-232
Nabam	AIII-234
Naled	AIII-236
Naphtha (solvent)	AIII-238
Naphthalene	AIII-240
α-Naphthalenesulfonic acid	AIII-242
β-Naphthalenesulfonic acid	AIII-244
α-Naphthol	AIII-246
β-Naphthol	AIII-248
1-Naphthylamine	AIII-250
2-Naphthylamine	AIII-252
Naptalam	AIII-254
Neopentanoic acid	AIII-256
Nitrilotriacetic acid, trisodium salt	AIII-258
p-Nitroaniline	AIII-260
Nitroanisole	AIII-262
Nitrobenzene	AIII-264

TABLE OF CONTENTS (Continued)

	Page
p-Nitrobenzoic acid	AIII-266
Nitrocellulose	AIII-268
Nitroethane	AIII-270
Nitroglycerine	AIII-272
Nitromethane	AIII-274
m-Nitrophenol	AIII-276
o-Nitrophenol	AIII-278
p-Nitrophenol	AIII-280
1-Nitropropane	AIII-282
2-Nitropropane	AIII-284
N-Nitrosodiethylamine	AIII-286
N-Nitrosodimethylamine	AIII-288
Nitrosoethylurea	AIII-290
Nitrosomethylurea	AIII-292
m-Nitrotoluene	AIII-294
o-Nitrotoluene	AIII-296
p-Nitrotoluene	AIII-298
Nonene	AIII-300
Nonyl phenol	AIII-302

APPENDIX III

CHEMISTRY, PRODUCTION AND TOXICITY OF SELECTED SYNTHETIC ORGANIC CHEMICALS

Ferbam

CHEMICAL NAME

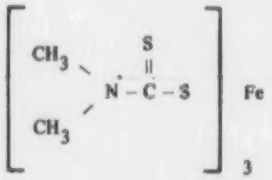
CAS Number: 301-05-3

Chemical Name: Ferbam

Synonyms: Dimethyldithiocarbamic acid
Ferric dimethyl dithiocarbamate
Tris (dimethyldithiocarbamato) iron

Molecular Formula: $C_9H_{18}FeN_3S_6$

Structure:



Chemical Properties

Molecular Weight:	416.5	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	Decomposes > 180°C
Density:		**Solubility:**	Slightly (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ferbam

PRODUCTION DATA

Annual U.S. Production: 2.3 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4000 mg/kg	rat	oral
	2700 mg/kg	rat	intraperitoneal
LD_{Lo}	63 mg/kg	mouse	intraperitoneal
	2000 mg/kg	rabbit	oral
	200 mg/kg	rabbit	intraperitoneal
	450 mg/kg	guinea pig	oral
	700 mg/kg	guinea pig	intraperitoneal

Non-lethal Acute Effects:
Irritant to eyes and mucous membranes

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 15 mg/m^3

Carcinogenicity: Recognized carcinogen

Mutagenicity:

Teratogenicity:

TLV: 15 mg/m^3

Other Chronic Effects:

Ferrocene

CHEMICAL NAME

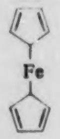
CAS Number: 102-54-5

Chemical Name: Ferrocene

Synonyms: Dicyclopentadiene iron

Molecular Formula: $C_{10}H_{10}Fe$

Structure:



Chemical Properties

Molecular Weight: 186.0

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: Sublimes

Melting Point: 173 to 174°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:
Resistant to ultraviolet light

Safety Hazard: Fire–moderate
Disaster hazard–dangerous–toxic fumes

Ferrocene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1320 mg/kg	rat	oral
	500 mg/kg	rat	intraperitoneal
	1550 mg/kg	mouse	oral
	335 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Fluometuron

CHEMICAL NAME

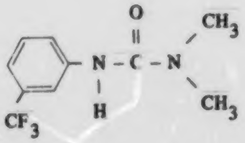
CAS Number: 2164-17-2

Chemical Name: 1,1-Dimethyl-3-(α,α,α-trifluoro-m-tolyl) urea

Synonyms: Fluometuron

Molecular Formula: $C_{10}H_{11}F_3N_2O$

Structure:



Chemical Properties

Molecular Weight:	232.23	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	163 to 164.5°C
Density:		**Solubility:**	90 ppm (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 4 x 10^6 lbs. (1971)

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	89 mg/kg	rat	oral
	900 mg/kg	mouse	oral

Non-lethal Acute Effects:

Emesis
Coma

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Depression

Folex

CHEMICAL NAME

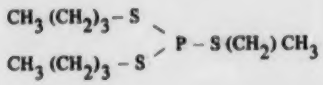
CAS Number: 150-50-5

Chemical Name: Phosphorotrithious acid, tributyl ester

Synonyms: Folex
S,S,S-Tributyl phosphorotrithioite

Molecular Formula: $C_{12}H_{27}PS_3$

Structure:



$$\begin{matrix} CH_3\,(CH_2)_3-S \\ CH_3\,(CH_2)_3-S \end{matrix} > P-S\,(CH_2)\,CH_3$$

Chemical Properties

Molecular Weight: 298.54

Vapor Pressure:

Boiling Point: 115 to 134°C at 0.08 mm

Density:

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 3×10^6 lbs. (1971)

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 3

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	910 mg/kg	rat	oral
	615 mg/kg	rat	skin
	76 mg/kg	rat	intraperitoneal
	350 mg/kg	rat	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Folpet

CHEMICAL NAME

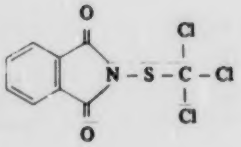
CAS Number: 133-07-3

Chemical Name: Phthalimide-N[(trichloromethyl)thio]

Synonyms: Folpet
Phaltan

Molecular Formula: $C_9H_4Cl_3NO_2S$

Structure:



Chemical Properties

Molecular Weight: 296.6

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient: 2.85

Physical State: Solid

Vapor Density:

Melting Point: 177°C

Solubility: Nearly insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous–emits highly toxic fumes of SO_X and NO_X

Folpet

PRODUCTION DATA

Annual U.S. Production: 2×10^6 lbs. (1971)

Consumption:

Fraction of Dispersion: Estimated at 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD$_{50}$	10,000 mg/kg	rat	oral
Non-lethal Acute Effects:			
TD$_{Lo}$	500 mg/kg (7 days)	pregnant hamster	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: Teratogenic

TLV:

Other Chronic Effects:

Formaldehyde

CHEMICAL NAME

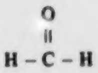
CAS Number: 50-00-0

Chemical Name: Formaldehyde (Commercial solutions 37%-50%)

Synonyms: Methanal
Methyl aldehyde
Formalin

Molecular Formula: CH_2O

Structure:



$$H-\overset{\overset{O}{\|}}{C}-H$$

Chemical Properties

Molecular Weight: 30.03

Vapor Pressure: 1946.67 mm at 25°C

Boiling Point: −21°C at 760 mm

Density: 0.815 at 20°C/4°C

Octanol/Water Partition Coefficient: −0.96

Physical State: Gas or Liquid

Vapor Density:

Melting Point: −92°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD: 30% of theoretical after 5 days at 20°C at 10 mg/ml
Total theoretical oxygen demand −1.1 gm/gm

Atmospheric Reactivity:
Activity toward O_3: No data
RO_2: $t_{1/2} = 10$ days
OH: $t_{1/2} = 1.2$ hours

Safety Hazard: Fire−moderate
Explosion−moderate

Formaldehyde

PRODUCTION DATA

Annual U.S. Production: 5651.8×10^6 lbs.

Consumption: 5622.8×10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 52.7

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD$_{50}$	420 mg/kg	rat	subcutaneous
	300 mg/kg	mouse	subcutaneous
	260 mg/kg	guinea pig	oral
LD$_{Lo}$	16 mg/kg	mouse	intraperitoneal
	36 mg/kg	human	oral
	550 mg/kg	dog	subcutaneous
	240 mg/kg	rabbit	subcutaneous
LC$_{Lo}$	900 mg/kg (2 hours)	mouse	inhalation
	820 mg/kg (8 hours)	cat	inhalation
Non-lethal Acute Effects:			
Irritant			
TC$_{Lo}$	13.8 ppm	human	inhalation
Conjunctivitis			
Dermatitis			

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 3 ppm
Ceiling limit 5 ppm
Peak exposure 10 ppm (30 minutes once in 8 hours)

Carcinogenicity:			
Spindle cell sarcomas		rats	injections
Neoplastic effects			
TD$_{Lo}$	1300 mg/kg (65 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV: 3 ppm

Other Chronic Effects:

Irritates eyes, respiratory tract and skin as low as 0.3 ppm

Formamide

CHEMICAL NAME

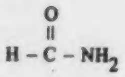
CAS Number: 75-12-7

Chemical Name: Formamide

Synonyms: Methaneamide

Molecular Formula: CH_3NO

Structure:



$$H-\overset{\overset{\displaystyle O}{\|}}{C}-NH_2$$

Chemical Properties

Molecular Weight: 45.04

Vapor Pressure: 1 mm at 70.5°C

Boiling Point: 210.7°C (decomposes starting at about 180°C)

Density: 1.134 at 20°C/4°C

Octanol/Water Partition Coefficient: -1.67

Physical State: Liquid

Vapor Density:

Melting Point: 2.55°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Disaster hazard–moderate–toxic fumes

Formamide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2539 mg/kg	guinea pig	intramuscular

Non-lethal Acute Effects:
Local irritant

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 20 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:
TD_{Lo} 6 gm/kg pregnant rat intraperitoneal

TLV:

Other Chronic Effects:

Formic acid

CHEMICAL NAME

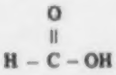
CAS Number: 64-18-6

Chemical Name: Formic acid

Synonyms: Methanoic acid
Hydrogen carboxylic acid

Molecular Formula: CH_2O_2

Structure:



$$H-\overset{\overset{O}{\|}}{C}-OH$$

Chemical Properties

Molecular Weight: 46.3

Physical State: Liquid

Vapor Pressure: 42.38 mm at 25°C

Vapor Density: 1.59

Boiling Point: 100.8°C

Melting Point: 8.3°C

Density: 1.2201 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: −0.73

Environmental Persistence

BOD: 68% of theoretical after 20 days at 20°C at 10 mg/ml
Total theoretical oxygen demand = 0.35 gm/gm

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

PRODUCTION DATA

Annual U.S. Production: 46.9 x 10^6 lbs.

Consumption: 46.9 x 10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 24.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1210 mg/kg	rat	oral
	1100 mg/kg	mouse	oral
	145 mg/kg	mouse	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects: Moderate effects as an irritant or upon inhalation
Severe effects following ingestion
Nausea–15 ppm

Fumaric acid

CHEMICAL NAME

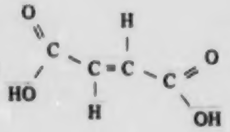
CAS Number: 110-17-8

Chemical Name: Fumaric acid

Synonyms: trans-Butenedioic acid
Boletic acid
Lichenic acid
Allomaleic acid

Molecular Formula: $C_4H_4O_4$

Structure:



Chemical Properties

Molecular Weight: 116.1

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 165°C at 1.7 mm (sublimes)

Melting Point: 287°C

Density: 1.635 at 20°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 0.56

Environmental Persistence

BOD: 82% of theoretical at 20° after 10 days
Total theoretical oxygen demand = 0.83 gm/gm

Atmospheric Reactivity:

Safety Hazard: Fire–slight

Fumaric acid

PRODUCTION DATA

Annual U.S. Production: 42×10^6 lbs. (1974)

Consumption: 42×10^6 lbs.

Fraction of Dispersion: 0.30

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 16.2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Furfural

CHEMICAL NAME

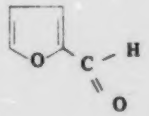
CAS Number: 98-01-1

Chemical Name: 2-Furaldehyde

Synonyms: 2-Furancarbonal
Furfural
Fural
Furale

Molecular Formula: $C_5H_4O_2$

Structure:



Chemical Properties

Molecular Weight: 96.1

Physical State: Liquid

Vapor Pressure: 2.08 mm at 25°C

Vapor Density: 3.31

Boiling Point: 161.7°C at 764 mm

Melting Point: −38.7°C

Density: 1.161 at 20°C/20°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–moderate

Furfural

PRODUCTION DATA

Annual U.S. Production: 149.6 x 10^6 lbs. (1974)

Consumption: 153 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	127 mg/kg	rat	oral
	425 mg/kg	mouse	oral
	2300 mg/kg	dog	oral
	928 mg/kg	rabbit	oral
	541 mg/kg	guinea pig	oral
LC_{Lo}	153 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Irritation to eyes, nose and throat

TD_{Lo} 600 gm/m^3 (eye)

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Furfuryl alcohol

CHEMICAL NAME

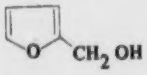
CAS Number: 98-00-0

Chemical Name: Furfuryl alcohol

Synonyms: 2-Furyl carbinol
(2-Furyl) methanol

Molecular Formula: $C_5H_6O_2$

Structure:



Chemical Properties

Molecular Weight:	98.1	**Physical State:**	Liquid
Vapor Pressure:	1 mm at 31.8°C	**Vapor Density:**	3.37
Boiling Point:	171°C at 750 mm	**Melting Point:**	
Density:	1.129 at 20°C/4°C	**Solubility:**	Infinite (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–moderate

Furfuryl alcohol

PRODUCTION DATA

Annual U.S. Production: Estimated as 70 x 10^6 lbs. (1974)

Consumption: 4 x 10^6 lbs. (1964)

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	275 mg/kg	rat	oral
	40 mg/kg	mouse	oral
	650 mg/kg	rabbit	intravenous
LC_{50}	233 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:
Irritation to eyes
Nausea

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects:

Glycerol

CHEMICAL NAME

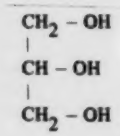
CAS Number: 56-81-5

Chemical Name: Glycerol

Synonyms: 1,2,3-Propane triol
Glycerin
Glycyl alcohol

Molecular Formula: $C_3H_8O_3$

Structure:



$$\begin{array}{l} CH_2-OH \\ \mid \\ CH-OH \\ \mid \\ CH_2-OH \end{array}$$

Chemical Properties

Molecular Weight: 92.09

Vapor Pressure: 4.99×10^{-4} at 25°C

Boiling Point: 290°C (decomposes)

Density: 1.2653 at 20°C/4°C

Octanol/Water Partition Coefficient: -2.66

Physical State: Liquid

Vapor Density: 3.17

Melting Point: 20°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD: 74% of theoretical for 10 days at 2 mg/l
Total theoretical oxygen demand = 1.37 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous

Glycerol

PRODUCTION DATA

Annual U.S. Production:	199.2×10^6 lbs.	**Consumption:**	144.1×10^6 lbs.
Fraction of Dispersion:	0.60	**Fraction of Production Lost:**	0.015

Release Rate (million lbs/yr): 89.4

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	7750 mg/kg	guinea pig	oral

Non-lethal Acute Effects:

Irritant to eyes and respiratory tract
Nausea and vomiting
Convulsions and paralysis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Glycerol monostearate

CHEMICAL NAME

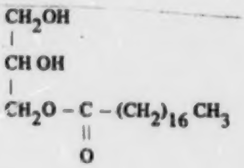
CAS Number: 1319-95-5

Chemical Name: Monostearin

Synonyms: Glyceryl monostearate
Glycerol monostearate
GMS

Molecular Formula: $C_{21}H_{42}O_4$

Structure:



$$\begin{array}{l} CH_2OH \\ \quad | \\ CH\,OH \\ \quad | \\ CH_2O-\underset{\underset{O}{\|}}{C}-(CH_2)_{16}CH_3 \end{array}$$

Chemical Properties

Molecular Weight: 358.63

Vapor Pressure:

Boiling Point: 58 to 59°C

Density: 0.97

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 74°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Glycerol monostearate

PRODUCTION DATA

Annual U.S. Production: 27.2×10^6 lbs.

Consumption: 27.2×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 28.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	200 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Glycidol

CHEMICAL NAME

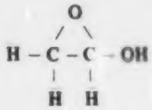
CAS Number: 556-52-5

Chemical Name: 2,3 – Epoxy – 1 – propanol

Synonyms: Glycide
Glycidol

Molecular Formula: $C_3H_6O_2$

Structure:



Chemical Properties

Molecular Weight: 74.09

Vapor Pressure:

Boiling Point: 167°C (decomposes)

Density: 1.165 at 0°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Infinite (H_2O)

Environmental Persistance

BOD:

Atmospheric Reactivity:

Safety Hazard:

Glycidol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	850 mg/kg	rat	oral
	450 mg/kg	mouse	oral
	1980 mg/kg	rabbit	skin
LC_{50}	580 ppm (8 hours)	rat	inhalation
	450 ppm (4 hours)	mouse	inhalation

Non-lethal Acute Effects:

Nervous excitation followed by depression
Irritant to eyes and respiratory tract

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 50 ppm

Other Chronic Effects:

Glycine

CHEMICAL NAME

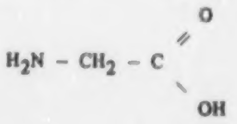
CAS Number: 56-40-6

Chemical Name: Glycine

Synonyms: Aminoacetic acid
Glycocoll

Molecular Formula: $C_2H_5NO_2$

Structure:



$H_2N - CH_2 - C(=O)OH$

Chemical Properties

Molecular Weight: 75.07

Vapor Pressure:

Boiling Point: (decomposes)

Density: 1.1607

Octanol/Water Partition Coefficient: -3.03

Physical State: Solid

Vapor Density:

Melting Point: 232 to 236°C (decomposes)

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Glyoxal

CHEMICAL NAME

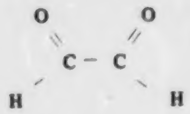
CAS Number: 107-22-2

Chemical Name: Glyoxal

Synonyms: Ethanedial
Oxalaldehyde
Biformyl

Molecular Formula: $C_2H_2O_2$

Structure:



Chemical Properties

Molecular Weight: 58.02

Vapor Pressure: <10 mm at 25°C

Boiling Point: 50.4°C

Density: 1.26 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid or Liquid

Vapor Density:

Melting Point: 15°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	200 mg/kg	mouse	intraperitoneal
	760 mg/kg	guinea pig	oral
	100 mg/kg	rat	oral

Non-lethal Acute Effects:
Local irritant to skin and mucous membranes

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Guanidine

CHEMICAL NAME

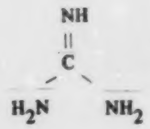
CAS Number: 113-00-8

Chemical Name: Guanidine

Synonyms: Amino methanamidine
Carbamamidine

Molecular Formula: CH_5N_3

Structure:



Chemical Properties

Molecular Weight: 59.07

Vapor Pressure:

Boiling Point: 160°C (decomposes)

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: ca. 50°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	175 mg/kg	rat	intraperitoneal
	300 mg/kg	mouse	subcutaneous
	200 mg/kg	dog	subcutaneous
	100 mg/kg	cat	intraperitoneal
	200 mg/kg	cat	subcutaneous
	500 mg/kg	rabbit	oral
	500 mg/kg	rabbit	subcutaneous
	1500 mg/kg	guinea pig	intraperitoneal
	100 mg/kg	guinea pig	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Guthion

CHEMICAL NAME

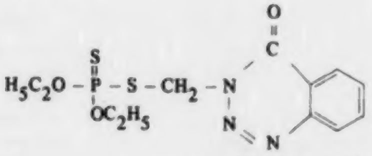
CAS Number: 86-50-0

Chemical Name: Phosphorodithioic acid, O-O, dimethyl ester, S-ester with 3-(mercaptomethyl)-1,2,3-benzotriazin-4(3H)-one

Synonyms:
Guthion
O-O-Dimethyl-S-(4-oxo-1,2,3-benzotriazin-3-(4H)-ylmethyl)-phosphorodithioate
Benzotriazinedithiophosphoric acid, dimethyoxy ester
N-Methylbenzamide, dimethyldiphosphoric acid ester

Molecular Formula: $C_{10}H_{12}N_3O_3PS_2$

Structure:



Chemical Properties

Molecular Weight: 317.34

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: Decomposes at elevated temperatures

Melting Point: 74°C

Density: 1.44

Solubility: Slightly (H_2O) (29 ppm at 25°C)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Guthion

PRODUCTION DATA

Annual U.S. Production: 4.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 4.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD$_{50}$	16 mg/kg	rat	oral
	300 mg/kg	rat	skin
	15 mg/kg	rat	unreported
	4 mg/kg	mouse	intraperitoneal
	80 mg/kg	guinea pig	oral
	277 mg/kg	chicken	oral
	8 mg/kg	wild bird	oral
LD$_{Lo}$	5 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA $200\ \mu g/m^3$ (skin)
EPA–Farm worker field reentry standard

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Cholinesterase inhibition

Heptachlor

CHEMICAL NAME

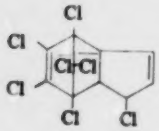
CAS Number: 76-44-8

Chemical Name: 1,4,5,6,7,8',8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methanoindene

Synonyms: Heptachlor
3,4,5,6,7,8,9-Heptachlorodicyclopentadiene

Molecular Formula: $C_{10}H_5Cl_7$

Structure:



Chemical Properties

Molecular Weight: 373.32

Vapor Pressure:

Boiling Point:

Density: 1.57 to 1.59

Octanol/Water Partition Coefficient: 5.05

Physical State: Solid

Vapor Density:

Melting Point: 95 to 96°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard–dangerous, decomposition to toxic fumes

Heptachlor

PRODUCTION DATA

Annual U.S. Production: 6 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 6.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	40 mg/kg	rat	oral
	195 mg/kg	rat	skin
	27 mg/kg	rat	intraperitoneal
	2000 mg/kg	rabbit	skin
	116 mg/kg	guinea pig	oral
Non-lethal Acute Effects:	62 mg/kg	chicken	oral
LD_{Lo}	25 mg/kg	mouse	oral
	40 mg/kg	mouse	intravenous

Convulsions
Kidney damage

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 500 $\mu g/m^3$ (skin)

Carcinogenicity:

Potential carcinogen according to EPA

Mutagenicity:

Teratogenicity:

TLV: 0.5 mg/m^3

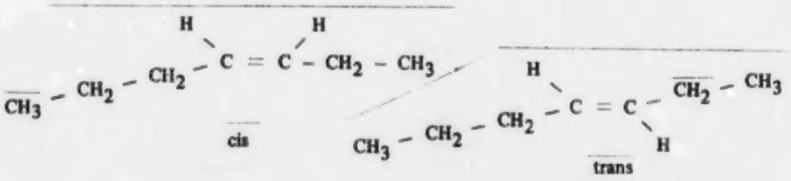
Other Chronic Effects:

Heptene

CHEMICAL NAME

CAS Number: cis: 7642-10-6
trans: 14686-14-7
Chemical Name: cis: (Z)-3-Heptene
trans: (E)-3-Heptene
Synonyms: 1-Ethyl-2-propyl ethylene
3-Heptene
3-Heptylene
Molecular Formula: C_7H_{14}

Structure:


H
H
CH3 – CH2 – CH2 – C = C – CH2 – CH3
cis
H
CH3 – CH2 – CH2 – C = C – CH2 – CH3
H
trans

Chemical Properties

Molecular Weight: 98.18

Physical State: Liquid

Vapor Pressure: 48.24 mm at 25°C

Vapor Density: 3.38

Boiling Point: 96°C at 760 mm (cis)
95.67°C at 760 mm (trans)

Melting Point: –136.63°C (trans)

Density: 0.7030 at 20°C/4°C (cis)
0.6981 at 20°C/4°C (trans)

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts vigorously with oxidizing materials

Safety Hazard: Fire–dangerous

PRODUCTION DATA

Annual U.S. Production: 114 x 10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Potential carcinogen according to EPA (unspecified isomer)

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Minor irritant
Minor effects upon ingestion or inhalation

Herban

CHEMICAL NAME

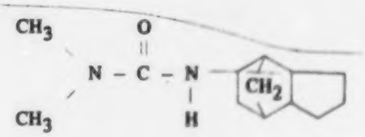
CAS Number: 2163-79-3

Chemical Name: 3-(Hexahydro-4,7-methanoindan-5-yl)-1,1-dimethyl urea

Synonyms: Herban
Norea

Molecular Formula: $C_{13}H_{22}N_2O$

Structure:



Chemical Properties

Molecular Weight: 222.3

Vapor Pressure: Insignificant

Boiling Point: Decomposes

Density: 1.162 at 25°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 168 to 169°C

Solubility: Very slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1470 mg/kg	rat	oral
	2000 mg/kg	rat	not reported
	4600 mg/kg	mouse	oral
	3700 mg/kg	dog	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

CHEMICAL NAME

CAS Number: 67-72-1

Chemical Name: Hexachloroethane

Synonyms: Carbon hexachloride
Perchloroethane

Molecular Formula: C_2Cl_6

Structure: $Cl_3C - CCl_3$

Chemical Properties

Molecular Weight: 236.76

Vapor Pressure: 1 mm at 32.7°C

Boiling Point: 186.6°C (sublimes)

Density: 2.091 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 185°C

Solubility: Insoluble (H_2O)

Environmental Persistance

BOD:

Atmospheric Reactivity:

Safety Hazard: Explosion–slight
Disaster hazard–when heated to decomposition, emits phosgene

Hexachloroethane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LC_{Lo}	325 mg/kg	dog	intravenous
	4000 mg/kg	rabbit	subcutaneous

Non-lethal Acute Effects:
Liver injury
Irritant to eyes
Mild narcosis

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 1 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

†TLV:

Other Chronic Effects:

Hexachloronaphthalene

CHEMICAL NAME

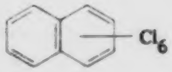
CAS Number: 1335-87-1

Chemical Name: Hexachloronaphthalene

Synonyms: Chloronaphthalene

Molecular Formula: $C_{10}H_2Cl_6$

Structure:



Chemical Properties

Molecular Weight:	334.9	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:	>288°C	**Melting Point:**	>88°C
Density:	>1.40 at 149°C	**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistance

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–chlorides

Hexachloronaphthalene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	11 mg/kg	cattle	oral

Non-lethal Acute Effects:

Acneform eruptions
Toxic narcosis of the liver

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 $\mu g/m^3$ (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Hexalene glycol

CHEMICAL NAME

CAS Number: 629-11-8

Chemical Name: 1,6-Hexanediol

Synonyms: Hexalene glycol
Hexamethylene glycol

Molecular Formula: $C_6H_{14}O_2$

Structure: $HO - CH_2 - (CH_2)_4 - CH_2OH$

Chemical Properties

Molecular Weight:	118.18	**Physical State:**	Liquid
Vapor Pressure:	<10 mm at 25°C	**Vapor Density:**	4.07
Boiling Point:	250°C at 760 mm	**Melting Point:**	41 to 42°C
Density:	0.967 at 0°C/4°C	**Solubility:**	Soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Hexalene glycol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3730 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Hexamethylenetetramine

CHEMICAL NAME

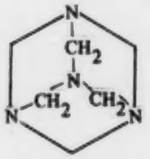
CAS Number: 100-97-0

Chemical Name: Hexamethylenetetramine

Synonyms:
Methenamine
Formamine
Hexamine
Urotropin
Metramine
Hexaform
Ammonioformaldehyde
Formin
Hexamethyleneamine
1,3,5,7-Tetraazaadamantane

Molecular Formula: $C_6H_{12}N_4$

Structure:



Chemical Properties

Molecular Weight: 140.19

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: Sublimes

Melting Point: 285 to 295°C

Density: 1.331 at -5°C

Solubility: Very soluble (666 gm/l H_2O)

Octanol/Water Partition Coefficient: -2.34

Environmental Persistence

BOD: 2% of theoretical after 5 days at 20°C
Total theoretical oxygen demand = 3.19 gm/gm

Atmospheric Reactivity:
Activity: reacts slowly with RO_2 and O_3
will react with oxidizing materials
Activity toward OH: $t_{1/2}$ = 9.6 hr.
Hydrolyzes rapidly at pH 3 or 7, $t_{1/2}$ = 1 day

Safety Hazard: Fire–Moderate

Hexamethylenetetramine

PRODUCTION DATA

Annual U.S. Production: 101 x 10^6 lbs.

Consumption: 101 x 10^6 lbs.

Fraction of Dispersion: 0.62

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 63.6

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	9200 mg/kg	rat	intravenous
	200 mg/kg	rat	subcutaneous
LD_{Lo}	512 mg/kg	mouse	intraperitoneal

Non-lethal Toxic Effects:
- Dermatitis
- Vesicular lesions

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic effects (sarcomas and adenomas):

TD_{Lo}	144 gm/kg (72 weeks)	rat	subcutaneous
Lymphomas		mouse	oral

Mutagenicity: Slight in mice, no details

Teratogenicity:

TLV:

Other Chronic Effects: Kidney damage

Hexanediamine

CHEMICAL NAME

CAS Number: 124-09-4

Chemical Name: 1,6-Hexanediamine

Synonyms: Hexamethylene diamine
HMDA

Molecular Formula: $C_6H_{16}N_2$

Structure: $H_2N - CH_2CH_2CH_2CH_2CH_2CH_2 - NH_2$

Chemical Properties

Molecular Weight: 116.21

Vapor Pressure:

Boiling Point: 205°C

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 39-42°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–Slight

Hexanediamine

PRODUCTION DATA

Annual U.S. Production: 613.4 x 10^6 lbs. (1970)

Consumption: 1224.4 x 10^6 lbs.

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 12.8

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
Irritation of eyes and mucous membranes			
Hepatitis			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Hydrogen cyanide

CHEMICAL NAME

CAS Number: 74-90-8

Chemical Name: Hydrocyanic acid

Synonyms: Hydrogen cyanide
Prussic acid

Molecular Formula: CHN

Structure: $HC \equiv N$

Chemical Properties

Molecular Weight:	27.03	**Physical State:**	Liquid
Vapor Pressure:	739.36 mm at 25°C	**Vapor Density:**	0.932
Boiling Point:	25.7°C at 760 mm	**Melting Point:**	-13.3°C
Density:	0.6876 at 20°C/4°C	**Solubility:**	Infinite (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Hydrogen cyanide

PRODUCTION DATA

Annual U.S. Production: 141.6 x 10^6 lbs. (1976 capacity)

Consumption: 365 x 10^6 lbs.

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3700 μg/kg	mouse	oral
	2990 μg/kg	mouse	intraperitoneal
	1100 μg/kg	mouse	intravenous
	2700 μg/kg	mouse	intramuscular
	1570 μg/kg	rabbit	intraperitoneal
	2500 μg/kg	rabbit	subcutaneous
	820 μg/kg	rabbit	intravenous
	1100 μg/kg	rabbit	intramuscular
LD_{Lo}	570 μg/kg	human	oral
	3 mg/kg	mouse	subcutaneous
	4 mg/kg	dog	oral
	1700 μg/kg	dog	subcutaneous
	2 mg/kg	cat	oral
	1100 μg/kg	cat	subcutaneous
	100 μg/kg	guinea pig	subcutaneous
LC_{50}	544 ppm (5 months)	rat	inhalation
	169 ppm (30 months)	mouse	inhalation
	300 ppm (3 months)	dog	inhalation
LC_{Lo}	120 mg/m^3 (1 hours)	human	inhalation
	2500 mg/m^3	cat	inhalation
	600 mg/m^3 (2 months)	rabbit	inhalation

Protoplasmic poison–halts cellular oxidation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects:

Hydroquinone

CHEMICAL NAME

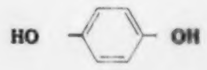
CAS Number: 123-31-9

Chemical Name: Hydroquinone

Synonyms:
p-Hydroquinone
1,4-Benzenediol
Quinol
Hydroquinol

Molecular Formula: C_6H_6O

Structure:



Chemical Properties

Molecular Weight: 110.6

Vapor Pressure: 1 mm at 132.4°C

Boiling Point: 286.2°C

Density: 1.358 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density: 3.81

Melting Point:

Solubility: Soluble (H_2O)

Environmental Persistence

BOD: 53% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Hydroquinone

PRODUCTION DATA

Annual U.S. Production: 29.7 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	370 mg/kg	cat	oral
	170 mg/kg	rat	intraperitoneal
	320 mg/kg	rat	oral
	115 mg/kg	rat	intravenous
	400 mg/kg	mouse	oral
	190 mg/kg	mouse	subcutaneous
	200 mg/kg	dog	oral
	70 mg/kg	cat	oral
	125 mg/kg	rabbit	intraperitoneal
	550 mg/kg	guinea pig	oral
	300 mg/kg	pigeon	oral
LD_{Lo}	200 mg/kg	rat	subcutaneous
	100 mg/kg	mouse	intraperitoneal
	150 mg/kg	guinea pig	intraperitoneal
	190 mg/kg	frog	parenteral

Non-lethal Acute Effects:

Dermatitis
Neurological effects
Jaundice
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Neoplastic:

TD_{Lo}	800 mg/kg	mouse	skin

Mutagenicity:

Teratogenicity:

TLV: 2 mg/m^3

Other Chronic Effects:

Indene

CHEMICAL NAME

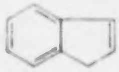
CAS Number: 95-13-6

Chemical Name: 1H-Indene

Synonyms: Indonaphthene
Indene
Inden

Molecular Formula: C_9H_8

Structure:



Chemical Properties

Molecular Weight: 116.2

Vapor Pressure: 2.23 mm at 25°C

Boiling Point: 182.6°C at 760 mm

Density: 0.9968 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -1.8 to -1.5°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Indene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Non-lethal Actue Effects:
Local irritant

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isoamyl alcohol

CHEMICAL NAME

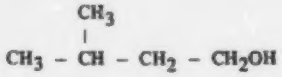
CAS Number: 123-51-3

Chemical Name: Isopentyl alcohol

Synonyms: Isoamyl alcohol, primary
Fusel oil
Isobutyl carbinol
3,3-Dimethyl-1-propanol

Molecular Formula: $C_5H_{12}O$

Structure:



$$CH_3 - \overset{\overset{CH_3}{|}}{CH} - CH_2 - CH_2OH$$

Chemical Properties

Molecular Weight: 88.15

Vapor Pressure: <10 mm at 25°C

Boiling Point: 132°C

Density: 0.813 at 15°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.04

Melting Point: -117.2°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–slight

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1300 mg/kg	rat	oral
	3970 mg/kg	rabbit	skin
LD_{Lo}	813 mg/kg	rat	intraperitoneal
	4250 mg/kg	rabbit	oral

Non-lethal Acute Effects:
Irritant to eyes and skin

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isobutyl acetate

CHEMICAL NAME

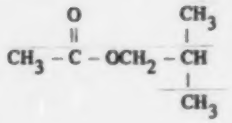
CAS Number: 110-19-0

Chemical Name: Acetic acid, isobutyl ester

Synonyms: Isobutyl acetate

Molecular Formula: $C_6H_{12}O_2$

Structure:



$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-OCH_2-\underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle CH_3}{|}}{CH}}$$

Chemical Properties

Molecular Weight: 116.2

Vapor Pressure: 19.61 mm at 25°C

Boiling Point: 118.0°C at 760 mm

Density: 0.8712 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.0

Melting Point: -99°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous

Isobutyl acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	4760 mg/kg	rabbit	oral
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:
Narcotic

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 150 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 150 ppm

Other Chronic Effects:

Isobutyl alcohol

CHEMICAL NAME

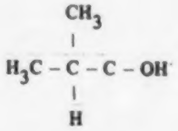
CAS Number: 78-83-1

Chemical Name: Isobutyl alcohol

Synonyms: 2-Methylpropanol
Isopropyl carbinol

Molecular Formula: C_4H_8O

Structure:



$$H_3C - \overset{\overset{\displaystyle CH_3}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - C - OH$$

Chemical Properties

Molecular Weight: 74.12

Vapor Pressure: 12.6 mm at 25°C

Boiling Point: 107.9

Density: 0.805 at 20°C/4°C

Octanol/Water Partition Coefficient: 0.97

Physical State: Liquid

Vapor Density: 2.55

Melting Point: -108°C

Solubility: Soluble (40 gm/l H_2O)

Environmental Persistence

BOD: 81% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 2.6 gm/gm

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–moderate
Disaster hazard–moderate–toxic fumes

Isobutyl alcohol

PRODUCTION DATA

Annual U.S. Production: 96.4 x 10^6 lbs.

Consumption: 96.4 x 10^6 lbs.

Fraction of Dispersion: 0.25

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 29.5

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2460 mg/kg	rat	oral
	4240 mg/kg	rabbit	skin
LD_{Lo}	3750 mg/kg	rabbit	oral
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

- Local irritant
- Conjunctivitis
- Dermatitis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Isobutyl aldehyde

CHEMICAL NAME

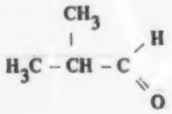
CAS Number: 78-84-2

Chemical Name: Isobutyraldehyde

Synonyms: Isobutyl aldehyde
2-Methyl propaldehyde
Isobutanal

Molecular Formula: C_4H_8O

Structure:



$H_3C-CH(CH_3)-CH=O$

Chemical Properties

Molecular Weight: 72.12

Vapor Pressure: 210 mm at 25°C

Boiling Point: 64°C

Density: 0.794 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -66°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Isobutylaldehyde

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2810 mg/kg	rat	oral
LC_{Lo}	8000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isobutylene

CHEMICAL NAME

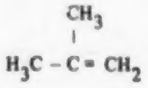
CAS Number: 115-11-7

Chemical Name: 2-Methyl-1-propene

Synonyms:
Isobutylene
Isobutene
2-Methylpropene

Molecular Formula: C_4H_8

Structure:



$$H_3C-\overset{\displaystyle CH_3}{\overset{|}{C}}=CH_2$$

Chemical Properties

Molecular Weight: 56.1

Vapor Pressure: 3290 mm at 40.5°C

Boiling Point: -6.9°C

Density: 0.600 at 20°C/4°C (liquid)

Octanol/Water Partition Coefficient:

Physical State: Liquid/liquified gas

Vapor Density: 1.94

Melting Point: -140.35°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–dangerous

Isobutylene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isobutyric acid

CHEMICAL NAME

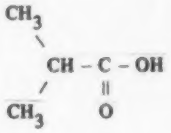
CAS Number: 79-31-2

Chemical Name: Isobutyric acid

Synonyms: 2-Methylpropanoic acid

Molecular Formula: $C_4H_8O_2$

Structure:



Chemical Properties

Molecular Weight: 88.1

Vapor Pressure: 2.67 mm at 25°C

Boiling Point: 153.2°C at 760 mm

Density: 0.949 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.00

Physical State: Liquid

Vapor Density: 3.04

Melting Point: –46.1°C

Solubility: Very Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	280 mg/kg	rat	oral
	500 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isodecyl alcohol

CHEMICAL NAME

CAS Number: (Mixture)

Chemical Name:

Synonyms: Isodecyl alcohol
isodecanol

Molecular Formula: $C_{10}H_{22}O$

Structure: Mixture of C_{10} alcohols, predominantly trimethyl heptanols

Chemical Properties

Molecular Weight: 158.32

Physical State: Liquid

Vapor Pressure: <.01 mm at 20°C

Vapor Density: 5.5

Boiling Point: 220.1°C

Melting Point:

Density: 0.8395

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 32% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 3.03 gm/gm.
Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Isodecyl alcohol

PRODUCTION DATA

Annual U.S. Production:	147×10^6 lbs.	**Consumption:**	147×10^6 lbs.
Fraction of Dispersion:	0.5	**Fraction of Production Lost:**	0.15

Release Rate (million lbs/yr): 75.7

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Isooctyl alcohol

CHEMICAL NAME

CAS Number: 26952-21-6

Chemical Name: Isooctanol

Synonyms: Isooctanol (isomer mix)

Molecular Formula: $C_8H_{18}O$

Structure: $(C_7H_{15})CH_2OH$

Chemical Properties

Molecular Weight: 130.26

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 182 to 195°C

Melting Point:

Density: 0.832 at 20°C/20°C

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Isooctyl alcohol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr): 15.8 (1972)

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1480 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isooctylphenol, ethoxylated

CHEMICAL NAME

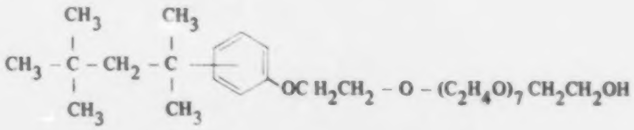
CAS Number: 11059-29-3

Chemical Name: 26-(Isooctylphenoxy)-3,6,9,12,15,18,21,24-octaoxahexacosan-1-ol

Synonyms: Octylphenol polyglycol ether
Isooctylphenoxypolyoxyethylene ethanol

Molecular Formula: $C_{32}H_{58}O_{10}$

Structure:



Chemical Properties

Molecular Weight:

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 150°C at 1 mm

Melting Point: 2 to 5°C

Density: 1.06 at 20°C

Solubility:

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–slight
Disaster hazard–dangerous–toxic fumes

Isooctylphenol, ethoxylated

PRODUCTION DATA

Annual U.S. Production: 20 x 10^6 lbs.

Consumption: 20 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 20.6

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}			
for x = 3	4000 mg/kg	rat	oral
x = 5	3800 mg/kg	rat	oral
x = 8-10	1800 mg/kg	rat	oral
x = 12-131	900 mg/kg	rat	oral
x = 16	2800 mg/kg	rat	oral
x = 20	3600 mg/kg	rat	oral

where x denotes the number of ethoxy groups

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isophorone

CHEMICAL NAME

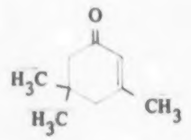
CAS Number: 78-59-1

Chemical Name: 3,5,5-Trimethyl-2-cyclohexen-1-one

Synonyms: Isophorone

Molecular Formula: $C_9H_{14}O$

Structure:



Chemical Properties

Molecular Weight: 138.1

Physical State: Liquid

Vapor Pressure: 1 mm at 38°C

Vapor Density: 4.77

Boiling Point: 215.2°C

Melting Point: -8.1°C

Density: 0.9229 at 20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Isophorone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2330 mg/kg	rat	oral

Non-lethal Acute Effects:

Local irritant
Lachrymation, opacity of cornea
Kidney poisoning

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm

Other Chronic Effects:

Isophthalic acid

CHEMICAL NAME

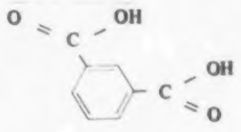
CAS Number: 121-91-5

Chemical Name: Isophthalic acid

Synonyms: Benzenedicarboxylic acid
Isophthalic acid

Molecular Formula: $C_8H_6O_4$

Structure:



Chemical Properties

Molecular Weight: 166.14

Vapor Pressure: <10 mm at 25°C

Boiling Point: Sublimes

Density: 1.593

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 348°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–slight

Isophthalic acid

PRODUCTION DATA

Annual U.S. Production: 100 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	4200 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isoprene

CHEMICAL NAME

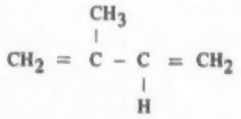
CAS Number: 78-79-5

Chemical Name: Isoprene

Synonyms: 2-Methyl-1,3-butadiene

Molecular Formula: C_5H_8

Structure:



$$CH_2 = \overset{CH_3}{\overset{|}{C}} - \underset{H}{\underset{|}{C}} = CH_2$$

Chemical Properties

Molecular Weight: 68.13

Vapor Pressure: 600.93 mm at 25°C

Boiling Point: 34°C at 760 mm

Density: 0.6806 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.35

Melting Point: -146°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–very dangerous

Isoprene

PRODUCTION DATA

Annual U.S. Production: 467×10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): e

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
Concentrations of 5% are fatal to mice			
LC_{Lo}	144 mg/m^3	mouse	inhalation
	180 mg/m^3	rat	inhalation

Non-lethal Acute Effects:

Irritant to eyes and mucous membranes

Anaesthesia at high concentration

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Isopropyl acetate

CHEMICAL NAME

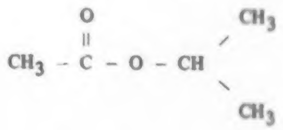
CAS Number: 108-21-4

Chemical Name: Acetic acid, 1-methyl ethyl ester

Synonyms: Isopropylacetate

Molecular Formula: $C_5H_{10}O_2$

Structure:



Chemical Properties

Molecular Weight: 102.13

Vapor Pressure: 58.8 mm at 25°C

Boiling Point: 90°C at 760 mm

Density: 0.8718 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.52

Melting Point: -73.4°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD: 13% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production: 41.9×10^6 lbs., 1967
(40×10^6 lbs., 1976 capacity)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 24.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC	3.2%	rat	--
TC_{Lo}	200 ppm	human	inhalation
LD_{50}	3000 mg/kg	rat	oral

Non-lethal Acute Effects:
Irritant to eyes, skin, and mucous membranes
Narcotic

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 250 ppm

Other Chronic Effects: Liver damage

Isopropyl alcohol

CHEMICAL NAME

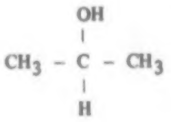
CAS Number: 67-63-0

Chemical Name: Isopropyl alcohol

Synonyms: 2-Propanol
sec-Propyl alcohol
Dimethylcarbinol

Molecular Formula: C_3H_8O

Structure:



$$CH_3 - \overset{\overset{\displaystyle OH}{|}}{\underset{\underset{\displaystyle H}{|}}{C}} - CH_3$$

Chemical Properties

Molecular Weight: 60.09

Physical State: Liquid

Vapor Pressure: 44.29 mm at 25°C

Vapor Density: 2.07

Boiling Point: 82.4°C at 760 mm

Melting Point: −89.5°C

Density: 0.7854 at 20°C/4°C

Solubility: Infinite (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 78% of theoretical after 20 days at 20°C
Total theoretical = 2.4 gm/gm

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

Isopropyl alcohol

PRODUCTION DATA

Annual U.S. Production: 1790×10^6 lbs.

Consumption: 1698.6×10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 876.2

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{100}	5000 mg/kg	rabbit	oral
	6000 mg/kg	mouse	subcutaneous
LD_{50}	933 mg/kg	mouse	intraperitoneal
	6000 mg/kg	dog	oral
	16 mg/kg	rabbit	skin
LD_{Lo}	2371 mg/kg	human	oral
	192 mg/kg	mouse	oral
	1963 mg/kg	cat	intravenous
	6 mg/kg	mammal	subcutaneous
Non-lethal Acute Effects:			
Conjunctivitis			
Anemia			
Irritant			
TC_{Lo}	400 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 400 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 400 ppm

Other Chronic Effects:

Isopropylamine

CHEMICAL NAME

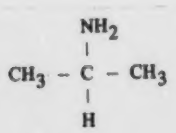
CAS Number: 75-31-0

Chemical Name: Isopropylamine

Synonyms: 2-Aminopropane

Molecular Formula: C_3H_9N

Structure:



$$CH_3 - \overset{\overset{NH_2}{|}}{\underset{\underset{H}{|}}{C}} - CH_3$$

Chemical Properties

Molecular Weight: 59.11

Vapor Pressure: 321.2 mm at 25°C

Boiling Point: 32.4°C at 760 mm

Density: 0.694 at 15°C/4°C

Octanol/Water Partition Coefficient: −0.13

Physical State: Liquid

Vapor Density: 2.03

Melting Point: -95.2°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD: 34% of theoretical after 10 days at 20°C

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous

Isopropylamine

PRODUCTION DATA

Annual U.S. Production: 18×10^6 lbs.

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	820 mg/kg	rat	oral
	550 mg/kg	rabbit	skin
LC_{Lo}	800 ppm (8 hours)	rat	inhalation
	7000 ppm (40 months)	mouse	inhalation

Non-lethal Acute Effects:

Strong irritant causing sensitivity of skin and mucous membranes
Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 5 ppm

Other Chronic Effects:

Isopropyl chloride

CHEMICAL NAME

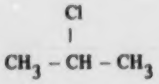
CAS Number: 75-29-6

Chemical Name: 2-Chloropropane

Synonyms: Isopropyl chloride
Isoprid

Molecular Formula: C_3H_7Cl

Structure:



$$CH_3 - \overset{\overset{\large Cl}{|}}{CH} - CH_3$$

Chemical Properties

Molecular Weight: 78.55

Vapor Pressure: 534.5 mm at 25°C

Boiling Point: 35.74°C at 760 mm

Density: 0.8617 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.71

Melting Point: -117.6°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–highly dangerous
Explosion–moderate
Disaster hazard–dangerous–toxic fumes–chlorides and phosgene

Isopropyl chloride

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Non-lethal Acute Effects:
Anaesthetic

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Isopropyl ether

CHEMICAL NAME

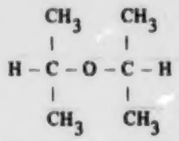
CAS Number: 108-20-3

Chemical Name: Isopropyl ether

Synonyms: 2-Isopropoxypropane
Diisopropyl ether

Molecular Formula: $C_6H_{14}O$

Structure:



$$\begin{array}{ccccccccc} & & CH_3 & & & & CH_3 & & \\ & & | & & & & | & & \\ H & - & C & - & O & - & C & - & H \\ & & | & & & & | & & \\ & & CH_3 & & & & CH_3 & & \end{array}$$

Chemical Properties

Molecular Weight: 102.17

Vapor Pressure: 150 mm at 25°C

Boiling Point: 68.5°C

Density: 0.719 at 25°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.52

Melting Point: -88°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–highly dangerous
Explosion–severe
Disaster hazard–dangerous–toxic fumes–peroxides

Isopropyl ether

PRODUCTION DATA

Annual U.S. Production: 14 x 10^6 lbs.

Consumption: 14 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 14.2

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	812 mg/kg	mouse	intraperitoneal
Non-lethal Acute Effects:			
Irritant			
TD_{Lo}	800 ppm (5 minutes)	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 500 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Narcotic at high concentrations

o-Isopropylphenol

CHEMICAL NAME

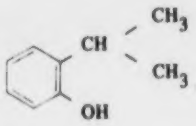
CAS Number: 88-69-7

Chemical Name: o-Isopropylphenol

Synonyms: 1-Hydroxy-2-isopropyl benzene
o-Cumenol

Molecular Formula: $C_9H_{12}O$

Structure:



Chemical Properties

Molecular Weight: 136.20

Vapor Pressure: 1 mm at 56.6°C

Boiling Point: 213 to 214°C at 760 mm

Density: 0.995 at 25°C/25°C

Octanol/Water Partition Coefficient: 1.08

Physical State: Liquid

Vapor Density:

Melting Point: 15 to 16°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Disaster hazard–dangerous–toxic fumes–phenol

o-Isopropylphenol

PRODUCTION DATA

Annual U.S. Production: 2084 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Isopropylphenol

CHEMICAL NAME

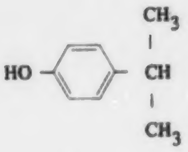
CAS Number: 99-89-8

Chemical Name: p-Isopropyl phenol

Synonyms: p-Cumenol
1-Hydroxy-4-isopropylphenol

Molecular Formula: $C_9H_{12}O$

Structure:



Chemical Properties

Molecular Weight:	136.2	**Physical State:**	Liquid
Vapor Pressure:	1 mm at 67°C	**Vapor Density:**	
Boiling Point:	228°C at 745 mm	**Melting Point:**	63.2°C
Density:	0.983	**Solubility:**	Slightly soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Disaster hazard—dangerous—toxic fumes—phenol

p-Isopropylphenol

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Ketene

CHEMICAL NAME

CAS Number: 463-51-4

Chemical Name: Ketene

Synonyms: Ethenone
Carbomethane
Keten

Molecular Formula: C_2H_2O

Structure: $CH_2=C=O$

Chemical Properties

Molecular Weight:	42.04	**Physical State:**	Gas
Vapor Pressure:		**Vapor Density:**	1.45
Boiling Point:	-56°C	**Melting Point:**	-151°C
Density:		**Solubility:**	Decomposes (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistance

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1300 mg/kg	rat	unreported
LC_{Lo}	23 ppm (30 minutes)	mouse	inhalation
	53 ppm (100 minutes)	rat	inhalation
	53 ppm (4 hours)	guinea pig	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 0.5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Pulmonary edema

Ligninsulfonic acid, ammonium salt

CHEMICAL NAME

CAS Number: Not listed in 9th Chemical Index

Chemical Name: (Complex mixture)

Synonyms: Ligninsulfonic acid, ammonium salt

Molecular Formula: (Complex mixture)

Structure: (Several structures are proposed)

Chemical Properties

Molecular Weight: 1,000 to 20,000

Vapor Pressure: Negligible at 25°C

Boiling Point: Decomposes above 200°C

Density: ca. 1.5

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ligninsulfonic acid, ammonium salt

PRODUCTION DATA

Annual U.S. Production:	40 x 10^6 lbs.	**Consumption:**	40 x 10^6 lbs.
Fraction of Dispersion:	0.98	**Fraction of Production Lost:**	0.03
Release Rate (million lbs/yr):	40.4		

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Ligninsulfonic acid, calcium salt

CHEMICAL NAME

CAS Number: (Not listed in 9th Chemical Index)

Chemical Name: (Complex mixture)

Synonyms: Ligninsulfonic acid, calcium salt

Molecular Formula: (Complex mixture)

Structure: (Several structures are proposed)

Chemical Properties

Molecular Weight:	(Unknown)	**Physical State:**	
Vapor Pressure:	Negligible	**Vapor Density:**	
Boiling Point:	Decomposes	**Melting Point:**	
Density:		**Solubility:**	Infinite (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ligninsulfonic acid, calcium salt

PRODUCTION DATA

Annual U.S. Production: 326.6 x 10 lbs.

Consumption: 326.6 x 10^6 lbs.

Fraction of Dispersion: 0.98

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 329.9

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ligninsulfonic acid, ferrochrome salt

CHEMICAL NAME

CAS Number: (Not listed in 9th Chemical Index)

Chemical Name: (Complex mixture)

Synonyms: Ligninsulfonic acid, ferrochrome salt

Molecular Formula: (Complex mixture)

Structure: (Several structures are proposed)

Chemical Properties

Molecular Weight:	(Unknown)	Physical State:	
Vapor Pressure:	Negligible	Vapor Density:	
Boiling Point:	Decomposes	Melting Point:	
Density:		Solubility:	Infinite
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ligninsulfonic acid, ferrochrome salt

PRODUCTION DATA

Annual U.S. Production: 60 x 10^6 lbs.

Consumption: 60 x 10^6 lbs.

Fraction of Dispersion: 0.98

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 60.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Ligninsulfonic acid, sodium salt

CHEMICAL NAME

CAS Number: Not listed in 9th Chemical Index

Chemical Name: (Complex mixture)

Synonyms: Ligninsulfonic acid, sodium salt

Molecular Formula: (Complex mixture)

Structure: (Several structures are proposed)

Chemical Properties

Molecular Weight:	(Unknown)	**Physical State:**	
Vapor Pressure:	Negligible at 25°C	**Vapor Density:**	
Boiling Point:	Decomposes	**Melting Point:**	
Density:		**Solubility:**	Infinite
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Ligninsulfonic acid, sodium salt

PRODUCTION DATA

Annual U.S. Production: 58.7 x 10^6 lbs.

Consumption: 58.7 x 10^6 lbs.

Fraction of Dispersion: 0.98

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 59.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Lindane

CHEMICAL NAME

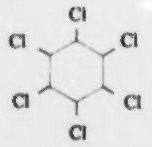
CAS Number: 58-89-9

Chemical Name: 1,2,3,4,5,6-Hexachlorocyclohexane (gamma isomer)

Synonyms: Gamma-benzene hexachloride
Gammexane

Molecular Formula: $C_6H_6Cl_6$

Structure:



Chemical Properties

Molecular Weight: 290.82

Physical State: Solid

Vapor Pressure: 0.0317 mm at 20°C

Vapor Density:

Boiling Point: 323.4°C at 760 mm

Melting Point: 112.5°C

Density:

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–phosgene

Lindane

PRODUCTION DATA

Annual U.S. Production: <1.0 x 10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): <1.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	88 mg/lg	rat	oral
	500 mg/lg	rat	skin
	86 mg/lg	mouse	oral
	60 mg/lg	rabbit	oral
	50 mg/lg	rabbit	skin
	127 mg/lg	guinea pig	oral
	180 mg/lg	child	oral
	840 mg/lg	human	oral
	35 mg/lg	rat	intraperitoneal
	75 mg/lg	mouse	intraperitoneal
	50 mg/lg	dog	oral
	8 mg/lg	dog	intravenous
	4000 μg/kg	rabbit	intravenous
	100 mg/kg	wild bird	oral
	26 mg/kg	wild bird	intramuscular

Non-lethal Acute Effects:

Local irritant–dermatitis
CNS stimulation--convulsions
Necrosis of blood vessels in lungs, liver and kidney
Pulmonary edema

Chronic Toxicity

U.S. Occupational Standard: (air) 500 mg/m^3 (skin)

Carcinogenicity:

Mutagenicity:

TD_{Lo} 29 gm/kg (52 weeks) mouse oral

Teratogenicity:

TLV:

Other Chronic Effects:

Linuron

CHEMICAL NAME

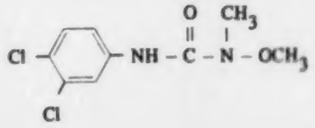
CAS Number: 330-55-2

Chemical Name: 3-(3,4-Dichlorophenyl)-1-methoxyl-1-methyl urea

Synonyms: Methoxy-1-methyl-3(3,4-dichlorophenyl)urea

Molecular Formula: $C_9H_{10}Cl_2N_2O_2$

Structure:



Chemical Properties

Molecular Weight: 249.11

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 93 to 94°C

Solubility: Slightly (H_2O) (75 ppm at 25°C)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Linuron

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1500 mg/kg	rat	unreported
	3300 mg/kg	rat	oral
	500 mg/kg	dog	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:
Irritant of nose, eyes, throat and skin

Magenta

CHEMICAL NAME

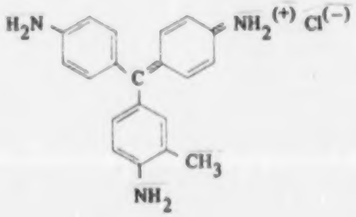
CAS Number: 3248-93-9

Chemical Name: 4-[(4-Aminophenyl)(4-imino-2,5-cyclohexadien-1-ylidene)methyl]-2-methyl benzenamine

Synonyms:
Magenta
Magenta I
Rosaniline
Fuchsin
α^4-(p-Aminophenyl)-α^4(4-imino-2,5-cyclohexadien-ylidene)-2,4-xylidene
2-Methyl-4,4'[(4-imino-2,5-cyclohexadien-1-ylidene)methylene] dianiline monohydrochloride

Molecular Formula: $C_{20}H_{19}N_3$

Structure:



Chemical Properties

Molecular Weight: 337.8

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 186°C (decomposes)

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Magenta

PRODUCTION DATA

Annual U.S. Production: 0.116 x 10^6 lbs. (1964)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	150 mg/kg	rabbit	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Recognized carcinogen

Neoplastic effects:

TD_{Lo}	2500 mg/kg (52 weeks)	mouse	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Malathion

CHEMICAL NAME

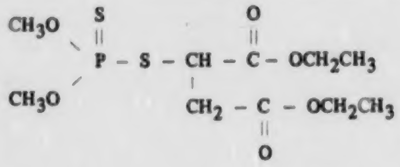
CAS Number: 121-75-5

Chemical Name: Mercapto-succinic acid, diethyl ester, S-ester with O,O-dimethyl phosophorodithioate

Synonyms: Malathion
O,O-Dimethyl-S-1,2-bis (ethoxy carbonyl) ethyl dithiophosphate

Molecular Formula: $C_{10}H_{19}O_6PS_2$

Structure:



Chemical Properties

Molecular Weight: 330.96

Vapor Pressure: 4×10^{-5} mm at 30°C

Boiling Point: 156°C at 77 mm

Density: 1.23 at 25°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: 2.85°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Malathion

PRODUCTION DATA

Annual U.S. Production: 30×10^6 lbs. (1972)

Consumption: 30×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 30.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	599 mg/kg	rat	oral
	340 mg/kg	rat	intraperitoneal
	50 mg/kg	rat	intravenous
	193 mg/kg	mouse	intraperitoneal
	500 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 15 mg/m^3 (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 15 mg/m^3

Other Chronic Effects: Allergic sensitization of skin

Maleic acid

CHEMICAL NAME

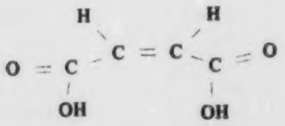
CAS Number: 110-16-7

Chemical Name: Maleic acid

Synonyms:
Maleinic acid
Toxilic acid
cis-Butenedioic acid

Molecular Formula: $C_4H_4O_4$

Structure:



$O=C(OH)-CH=CH-C(OH)=O$

Chemical Properties

Molecular Weight: 116.07

Vapor Pressure: Essentially O

Boiling Point: 135°C–decomposes

Density: 1.590 at 20°C/4°C

Octanol/Water Partition Coefficient: –0.79

Physical State: Solid

Vapor Density: 4.0

Melting Point: 139 to 140°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity.
Stable to ultraviolet irradiation

Safety Hazard: Fire–slight

PRODUCTION DATA

Annual U.S. Production: 283.2 x 10^6 lbs. (1974)

Consumption: ca. 283.2 x 10^6 lbs.

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	708 mg/kg	rat	oral
	1560 mg/kg	rabbit	skin

Non-lethal Acute Effects:

- Irritant
- Hypofunction of glycogen synthesis in liver
- Conjunctivitis
- Dermatitis

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Maleic anhydride

CHEMICAL NAME

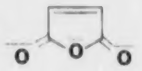
CAS Number: 108-31-6

Chemical Name: Maleic anhydride

Synonyms: Toxilic anhydride
cis Butene dioicanhydride

Molecular Formula: $C_4H_2O_3$

Structure:



Chemical Properties

Molecular Weight:	98.06	**Physical State:**	Solid
Vapor Pressure:	1 mm at 44°C	**Vapor Density:**	3.4
Boiling Point:	197 to 199°C	**Melting Point:**	60°C
Density:	1.48 at 20°C/4°C	**Solubility:**	Reacts with water; Soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing agents

Safety Hazard: Fire: moderate–toxic fumes

Maleic anhydride

PRODUCTION DATA

Annual U.S. Production: 211.8×10^6 lbs. (1975)

Consumption: 230×10^6 lbs. (1975)

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 4.72

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	60 mg/kg	mouse	oral
LD_{Lo}	850 mg/kg	rat	oral

Non-lethal Acute Effects:

Burns to eyes and skin
Pulmonary edema

Chronic Toxicity

U.S. Occupational Standard: (air): TWA 0.25 ppm

Carcinogenicity:

TD_{Lo}	610 mg/kg (61 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV: 0.25 ppm

Other Chronic Effects:

Maleic hydrazide

CHEMICAL NAME

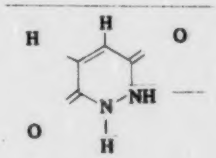
CAS Number: 123-33-1

Chemical Name: 1,2-Dihydro-3,6-pyridazinedione

Synonyms: Maleic hydrazide
3,6-Dioxo-1,2,3,6-tetrahydropyridazine

Molecular Formula: $C_4H_4N_2O_2$

Structure:



Chemical Properties

Molecular Weight:	112.09	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	>300°C decomposes
Density:		**Solubility:**	Slightly soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire: Dangerous—toxic fumes

Maleic hydrazide

PRODUCTION DATA

Annual U.S. Production: 3 x 10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 3.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3800 mg/kg	rat	oral
LD_{Lo}	8800 mg/kg	mouse	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: (suspected)

TD_{Lo}	1300 mg/kg (65 weeks)	rat	subcutaneous
	8800 mg/kg (3 weeks)	mouse	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Malic acid

CHEMICAL NAME

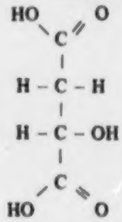
CAS Number: (dl): 617-48-1
(d): 636-61-3
(l): 97-67-6

Chemical Name: DL - Malic acid
D - Malic acid
L - Malic acid

Synonyms: Hydroxysuccinic acid
Apple acid

Molecular Formula: $C_4H_6O_5$

Structure:



Chemical Properties

Molecular Weight: 134.09

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 150°C (dl) (decomposes)
140°C (d and l) (decomposes)

Melting Point: 128°C (dl)
100°C (d and l)

Density: 1.601 at 20°C/4°C (dl)
1.595 at 20°C/4°C (d and l)

Solubility: Very soluble (H_2O)

Octanol/Water Partition Coefficient: -1.53

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
Unspecified optical isomer			
LD_{Lo}	1600 mg/kg	rat	oral
L (+) isomer			
LD_{Lo}	5000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Melamine

CHEMICAL NAME

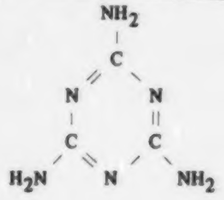
CAS Number: 108-78-1

Chemical Name: Melamine

Synonyms: 2,4,6-Triamine-S-triazine
Cyanurotriamide
2,4,6-Triamino-1,3,5-triazine

Molecular Formula: $C_3H_6N_6$

Structure:



Chemical Properties

Molecular Weight:	126.13	**Physical State:**	Solid
Vapor Pressure:	50 mm at 315°C	**Vapor Density:**	4.34
Boiling Point:	Sublimes	**Melting Point:**	354°C (decomposes)
Density:	1.573 at 20°C/4°C	**Solubility:**	Slightly soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster Hazard: Dangerous–toxic fumes–cyanides

Melamine

PRODUCTION DATA

Annual U.S. Production: 170×10^6 lbs (1973)

Consumption: 110×10^6 lbs. (1975)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	1600 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Mesitylene

CHEMICAL NAME

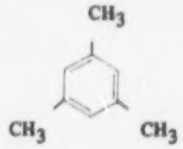
CAS Number: 95-63-6

Chemical Name: 1,3,4-Trimethyl benzene

Synonyms: Mesitylene

Molecular Formula: C_9H_{12}

Structure:



Chemical Properties

Molecular Weight: 120.21

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 164.7°C at 760 mm

Melting Point: -44.7°C

Density: 0.8637 at 20°C/4°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Mesitylene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LC_{Lo}	2400 ppm (24 hours)	rat	inhalation
LD_{Lo}	1500 mg/kg	rat	intraperitoneal
	1303 mg/kg	guinea pig	intraperitoneal

Non-lethal Acute Effects:

Narcotic leucopenia and thrombocytopenia
Dermatitis and conjunctivitis
Central nervous system:

TC_{Lo}	10 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Mesityl oxide

CHEMICAL NAME

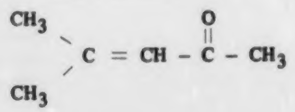
CAS Number: 141-79-7

Chemical Name: 4-Methyl-3-penten-2 one

Synonyms: Mesityl oxide

Molecular Formula: $C_6H_{10}O$

Structure:



$$\begin{matrix} CH_3 \\ \\ CH_3 \end{matrix}\!\!\!\begin{matrix} \diagdown \\ \\ \diagup \end{matrix} C = CH - \overset{\overset{\displaystyle O}{\|}}{C} - CH_3$$

Chemical Properties

Molecular Weight: 98.14

Physical State: liquid

Vapor Pressure: 9.16 mm at 25°C

Vapor Density: 3.38

Boiling Point: 130°C at 760 mm

Melting Point: –52.85°C

Density: 0.8653 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient: 1.24

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing material

Safety Hazard: Fire–Moderate

Mesityl oxide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1120 mg/kg	rat	oral
	354 mg/kg	mouse	intraperitoneal
	1000 mg/kg	rabbit	oral
LC_{Lo}	1000 ppm (4 hours)	rat	inhalation
LD_{Lo}	1000 mg/kg	rat	intraperitoneal

Non-lethal Acute Effects:

Local irritant
Causes opaque cornea
Keratoconus
Extensive necrosis of the cornea
Liver and kidney effects
Damage to lungs

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm

Other Chronic Effects:

Methacrylic acid

CHEMICAL NAME

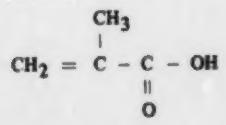
CAS Number: 79-41-4

Chemical Name: Methacrylic acid

Synonyms: α-Methyl acrylic acid
2-Methyl propenoic acid

Molecular Formula: $C_4H_6O_2$

Structure:



$$\mathrm{CH_2 = \overset{CH_3}{\overset{|}{C}} - \underset{\underset{O}{\|}}{C} - OH}$$

Chemical Properties

Molecular Weight: 86.1

Vapor Pressure: 1 mm at 25.5°C

Boiling Point: 162 to 163°C at 757 mm

Density: 1.0153 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: 16°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Disaster Hazard: dangerous–toxic fumes

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	49mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:
Local irritant to eyes and trachea

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methacrylonitrile

CHEMICAL NAME

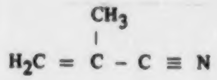
CAS Number: 126-98-7

Chemical Name: Methacrylonitrile

Synonyms: 2-Methylpropenitrile
Isopropene cyanide

Molecular Formula: C_4H_5N

Structure:



$$H_2C = \overset{\overset{\displaystyle CH_3}{|}}{C} - C \equiv N$$

Chemical Properties

Molecular Weight: 67.09

Vapor Pressure: 72.38 mm at 25°C

Boiling Point: 90.3°C at 760 mm

Density: 0.7998 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -35.8°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methacrylonitrile

PRODUCTION DATA

Annual U.S. Production: 10 x 10^6 lbs. (1967 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	250 mg/kg	rat	oral
	320 mg/kg	rabbit	skin
LD_{Lo}	15 mg/kg	mouse	oral
	65 mg/kg	mouse	intraperitoneal
LC_{50}	328 ppm (4 hours)	rat	inhalation
	36 ppm (4 hours)	mouse	inhalation
	37 ppm (4 hours)	rabbit	inhalation
	80 ppm (4 hours)	guinea pig	inhalation

Non-lethal Acute Effects:
Dermatitis
Lachrymation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects: Highly toxic following skin absorption or inhalation

Methallyl alcohol

CHEMICAL NAME

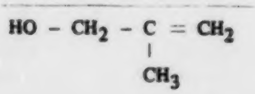
CAS Number: 513-42-8

Chemical Name: 2-Methyl-2-propen-1-ol

Synonyms: Methallyl alcohol
Methallyl hydroxide

Molecular Formula: C_4H_8O

Structure:



$$HO - CH_2 - \underset{\substack{| \\ CH_3}}{C} = CH_2$$

Chemical Properties

Molecular Weight: 72.12

Vapor Pressure:

Boiling Point: 114.49°C

Density: 0.8540 at 20°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methallyl alcohol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	500 mg/kg	mouse	oral
	2000 mg/kg	rabbit	skin
LC_{Lo}	2924 ppm (2 hours)	mouse	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methallyl chloride

CHEMICAL NAME

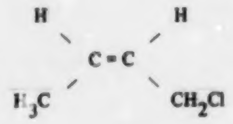
CAS Number: 563-47-3

Chemical Name: 3-Chloro-2-methyl propene

Synonyms: 2-Butene-1-chloride
1-Chloro-2-butene(cis)
β-Methallyl chloride

Molecular Formula: C_4H_7Cl

Structure:



Chemical Properties

Molecular Weight: 90.55

Vapor Pressure: 101.7 mm at 20°C

Boiling Point: 84.1°C at 758 mm

Density: 0.9426 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.12

Melting Point:

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–dangerous
Explosion–moderate
Disaster hazard–dangerous–toxic fumes–chlorides

Methallyl chloride

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LC_{50}	2000 mg/m^3 (24 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methane

CHEMICAL NAME

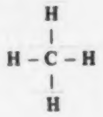
CAS Number: 74-82-8

Chemical Name: Methane

Synonyms: Marsh gas
Methyl hydride

Molecular Formula: CH_4

Structure:



$$\begin{array}{c} H \\ | \\ H-C-H \\ | \\ H \end{array}$$

Chemical Properties

Molecular Weight: 16.04

Vapor Pressure:

Boiling Point: −164°C at 760 mm

Density: 0.415 at −165°C

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density: 0.6

Melting Point: −182.48°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:
Residence in atmosphere: 4 to 7 years

Safety Hazard:

Methane

PRODUCTION DATA

Annual U.S. Production: 12,400 × 10^6 lbs (1964)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LC_{50}	400 ppm	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methanearsonic acid

CHEMICAL NAME

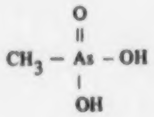
CAS Number: 124-58-3

Chemical Name: Methanearsonic acid

Synonyms: Methyl arsonic acid

Molecular Formula: CH_5AsO_3

Structure:



$$CH_3-\overset{\overset{\displaystyle O}{\|}}{\underset{\underset{\displaystyle OH}{|}}{As}}-OH$$

Chemical Properties

Molecular Weight: 139.97

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 160 to 161°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methanearsonic acid

PRODUCTION DATA

Annual U.S. Production:	30.7 x 10^6 lbs.	**Consumption:**	30.7 x 10^6 lbs.
Fraction of Dispersion:	1.0	**Fraction of Production Lost:**	0.01

Release Rate (million lbs/yr): 31

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3350 mg/kg	mouse	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

Methomyl

CHEMICAL NAME

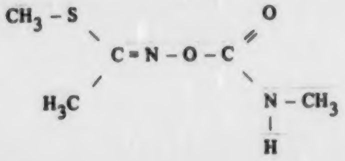
CAS Number: 16752-77-5

Chemical Name: N-([(Methylamino)carbonyl] oxy)ethanimidothioic acid, methyl ester

Synonyms: S-Methyl-N-[(methylcarbamoyl)-oxy] -thioacetimidate

Molecular Formula: $C_5H_{10}N_2O_2S$

Structure:



Chemical Properties

Molecular Weight:	162.23	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	78 to 79°C
Density:		**Solubility:**	
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methomyl

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	17 mg/kg	rat (male)	oral
	24 mg/kg	rat (female)	oral
	15 mg/kg	duck	oral
	10 mg/kg	wild bird species	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methoxychlor

CHEMICAL NAME

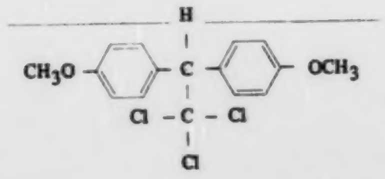
CAS Number: 72-43-5

Chemical Name: 1,1,1-Trichloro-2,2-bis(p-methoxyphenyl) ethane

Synonyms: DMDT
2,2-bis(p-Methoxyphenyl)-1,1,1-trichloroethane
Methoxychlor

Molecular Formula: $C_{16}H_{15}Cl_3O_2$

Structure:



Chemical Properties

Molecular Weight: 345.7

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density: 12

Melting Point: 94°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:
Slight air contaminant

Safety Hazard: Disaster hazard: Dangerous–toxic fumes–chlorides

Methoxychlor

PRODUCTION DATA

Annual U.S. Production:: 10.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 10.0

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	5000 mg/kg	rat	oral
	6430 mg/kg	human	oral
LD_{Lo}	2414 mg/kg	human skin	unspecified toxic effects

Non-lethal Acute Effects:
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 15 mg/m^3

Carcinogenicity:
Neoplastic effects
1100 mg/kg (36 weeks) rat oral

Mutagenicity:

Teratogenicity:

TLV: 15 mg/m^3

Other Chronic Effects: Kidney injury

Methoxyethanol

CHEMICAL NAME

CAS Number: 109-86-4

Chemical Name: 2-Methoxy ethanol

Synonyms: Methyl glycol
Methoxy hydroxy ethane
Methyl cellosolve

Molecular Formula: $C_3H_8O_2$

Structure: $CH_3 - O - CH_2 - CH_2 - OH$

Chemical Properties

Molecular Weight: 76.09

Vapor Pressure: 6.2 mm at 20°C

Boiling Point: 124.6°C

Density: 0.9660 at 20°C/4°C

Octanol/Water Partition Coefficient: −0.82

Physical State: Liquid

Vapor Density: 2.62

Melting Point: −85.1°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD: 88% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 1.68 gm/gm

Atmospheric Reactivity:
Reacts with oxidizing materials

Safety Hazard: Fire–Moderate

Methoxyethanol

PRODUCTION DATA

Annual U.S. Production: 119.1 x 10^6 lbs.

Consumption: 106.1 x 10^6 lbs.

Fraction of Dispersion: 0.26

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 29.4

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2460 mg/kg	rat	oral
	2140 mg/kg	rat	intravenous
	890 mg/kg	rabbit	oral
	1340 mg/kg	rabbit	skin
	950 mg/kg	guinea pig	oral
LD_{Lo}	3570 mg/kg	human	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation
Non-lethal Acute Effects:			
Aplastic anemia			
TC_{Lo}	25 ppm	human (CNS)	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl acetate

CHEMICAL NAME

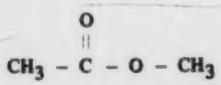
CAS Number: 79-20-9

Chemical Name: Acetic acid, methyl ester

Synonyms: Methyl acetate

Molecular Formula: $C_3H_6O_2$

Structure:



$$CH_3 - \overset{\overset{O}{\parallel}}{C} - O - CH_3$$

Chemical Properties

Molecular Weight: 74.08

Vapor Pressure: 212.5 mm at 25°C

Boiling Point: 57.8°C

Density: 0.9330 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.55

Melting Point: -98.1°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire: dangerous
Explosion: moderate

Methyl acetate

PRODUCTION DATA

Annual U.S. Production: 8.8 x 10^6 lbs. (1966)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3700 mg/kg	rabbit	oral
LD_{Lo}	4800 mg/kg	rat	oral
	3000 mg/kg	rat	subcutaneous
	3000 mg/kg	guinea pig	subcutaneous
LC_{Lo}	80 mg/m^3 (31 minutes)	mouse	inhalation
	67 mg/m^3 (56 minutes)	cat	inhalation

Non-lethal Acute Effects:

Narcotic

Irritant to eyes and mucous membranes (10,000 ppm)

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm

Other Chronic Effects:

Methyl acetoacetate

CHEMICAL NAME

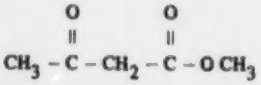
CAS Number: 105-45-3

Chemical Name: Acetoacetic acid, methyl ester

Synonyms: Methyl acetylacetonate

Molecular Formula: $C_5H_8O_3$

Structure:



$$CH_3-\overset{\overset{\displaystyle O}{\|}}{C}-CH_2-\overset{\overset{\displaystyle O}{\|}}{C}-OCH_3$$

Chemical Properties

Molecular Weight: 116.05

Vapor Pressure: 0.7 mm at 20°C

Boiling Point: 171.7°C

Density: 1.0785 at 20°C/20°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -31.9°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methyl acetoacetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylal

CHEMICAL NAME

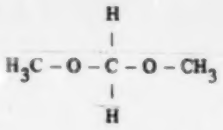
CAS Number: 109-87-5

Chemical Name: Dimethoxymethane

Synonyms:
Formal
Methylene dimethyl ether
Methylal
Formaldehyde dimethyl acetal

Molecular Formula: $C_3H_8O_2$

Structure:



$$H_3C-O-\overset{H}{\underset{H}{C}}-O-CH_3$$

Chemical Properties

Molecular Weight: 76.1

Vapor Pressure: 330 mm at 20°C

Boiling Point: 45.5°C at 760 mm

Density: 0.8593 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.63

Melting Point: -104.8°C

Solubility: Soluble (H_2O)

Environmental Persistance

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	3013 mg/kg	guinea pig	subcutaneous

Non-lethal Acute Effects:

Injury to lungs, kidney, liver and heart
Narcotic in high concentration

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1000 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1000 ppm

Other Chronic Effects:

Methyl alcohol

CHEMICAL NAME

CAS Number: 67-56-1

Chemical Name: Methanol

Synonyms: Methyl alcohol
Carbinol
Methyl hydroxide

Molecular Formula: CH_4O

Structure: CH_3OH

Chemical Properties

Molecular Weight:	32.04	**Physical State:**	Liquid
Vapor Pressure:	127.9 mm at 25°C	**Vapor Density:**	1.11
Boiling Point:	64.8°C	**Melting Point:**	-93.9°C
Density:	0.7913 at 20°C/4°C	**Solubility:**	Infinite (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD: 95% of theoretical at 20°C for 20 days
Total theoretical oxygen demand = 1.5 gm/gm

Atmospheric Reactivity:
Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

Methyl alcohol

PRODUCTION DATA

Annual U.S. Production: 5103.5×10^6 lbs. (1975)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 987.7

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	9800 mg/kg	mouse	subcutaneous
LD_{Lo}	340 mg/kg	human	oral
	1800 mg/kg	rat	intraperitoneal
	420 mg/kg	mouse	oral
	6300 mg/kg	dog	oral
	7000 mg/kg	donkey	oral
	4750 mg/kg	rabbit	oral
LC_{50}	1000 ppm	monkey	inhalation
Non-lethal Acute Effects:			
Eye-irritant, blindness			
TD_{Lo}	100 mg/kg	human	oral
CNS narcotic			
TD_{Lo}	300 ppm	human	inhalation

Irritant to mucous membranes; drying of skin; dermatitis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 200 ppm
Odor perception: 5,900 ppm

Other Chronic Effects:
- Conjunctivitis
- Headache
- Giddyness
- Insomnia
- Gastric disturbances
- Failure of vision–300 ppm

Methylamine

CHEMICAL NAME

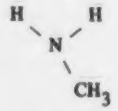
CAS Number: 74-89-5

Chemical Name: Methylamine

Synonyms: Monomethylamine
Aminomethane

Molecular Formula: CH_5N

Structure:



Chemical Properties

Molecular Weight: 31.1

Vapor Pressure: 2509 mm at 25°C

Boiling Point: -6.3°C at 760 mm

Density: 0.662 at 20°C/4°C

Octanol/Water Partition Coefficient: -1.00

Physical State: Gas

Vapor Density: 1.07

Melting Point: -93.5°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

Methylamine

PRODUCTION DATA

Annual U.S. Production: 319 x 10^6 lbs (1976 capacity)

Consumption: 185 x 10^6 lbs. (1975-all methyl amines)

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3000 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:
Strong irritant

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylamyl acetate

CHEMICAL NAME

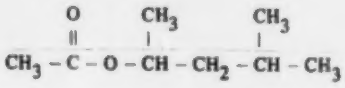
CAS Number: 108-84-9

Chemical Name: 4-Methyl-2-pentanol, acetate

Synonyms: 4-Methyl-2-pentyl acetate
Acetic acid, 1,3-dimethylbutyl ester
Methylisobutylcarbinol acetate

Molecular Formula: $C_8H_{16}O_2$

Structure:



$$CH_3-\overset{\overset{O}{\|}}{C}-O-\overset{\overset{CH_3}{|}}{CH}-CH_2-\overset{\overset{CH_3}{|}}{CH}-CH_3$$

Chemical Properties

Molecular Weight: 144.21

Vapor Pressure: 3. mm at 20°C

Boiling Point: 147 to 148°C

Density: 0.8805 at 0°C/0°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.97

Melting Point: -63.8°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire--moderate

Methylamyl acetate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	4000 ppm	rat	inhalation
Non-lethal Acute Effects:			
Eye irritation:			
LC_{Lo}	100 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 50 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylamyl alcohol

CHEMICAL NAME

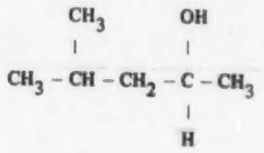
CAS Number: 108-11-2

Chemical Name: 4-Methyl-2-pentanol

Synonyms: Methyl isobutyl carbinol
Methyl amyl alcohol

Molecular Formula: $C_6H_{14}O$

Structure:



$$\begin{array}{ccccccccc} & & \mathrm{CH_3} & & & & \mathrm{OH} & & \\ & & | & & & & | & & \\ \mathrm{CH_3} & - & \mathrm{CH} & - & \mathrm{CH_2} & - & \mathrm{C} & - & \mathrm{CH_3} \\ & & & & & & | & & \\ & & & & & & \mathrm{H} & & \end{array}$$

Chemical Properties

Molecular Weight: 102.18

Vapor Pressure: 2.8 mm at 20°C

Boiling Point: 133°C at 760 mm

Density: 0.8075 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.53

Melting Point: -90°C (sets)

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

Methylamyl alcohol

PRODUCTION DATA

Annual U.S. Production: 50 x 10^6 lbs.

Consumption: 50 x 10^6 lbs.

Fraction of Dispersion: 0.80

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 40.8

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	812 mg/kg	mouse	intraperitoneal
	3560 mg/kg	rabbit	skin
	2600 mg/kg	rat	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Local irritant

Anesthetic in high concentrations

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 25 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylaniline

CHEMICAL NAME

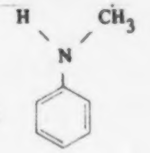
CAS Number: 100-61-8

Chemical Name: N-Methyl aniline

Synonyms: Monomethyl aniline
Methyl phenylamine

Molecular Formula: C_7H_9N

Structure:



Chemical Properties

Molecular Weight: 107.15

Vapor Pressure: 1 mm at 36°C

Boiling Point: 196.25°C at 760 mm

Density: 0.98912 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.82

Physical State: Liquid

Vapor Density: 3.70

Melting Point: -57°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Disaster hazard—dangerous—toxic fumes—aniline

Methylaniline

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	24 mg/kg	cat	intravenous
	280 mg/kg	rabbit	oral
	24 mg/kg	rabbit	intravenous
	1200 mg/kg	guinea pig	oral
	1200 mg/kg	guinea pig	subcutaneous

Non-lethal Acute Effects:

- Allergen
- Hemorrhage in bladder
- Nervous disorders

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 2 ppm

Carcinogenicity: Carcinogen

Neoplastic Effects:

TD_{Lo}	380 mg/kg (28 weeks)	mouse	oral

Mutagenicity:

Teratogenicity:

TLV: 2 ppm (skin)

Other Chronic Effects:

Methylbenzyl alcohol

CHEMICAL NAME

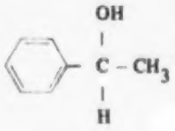
CAS Number: 98-85-1

Chemical Name: α-Methylbenzyl alcohol

Synonyms:
Methyl phenyl carbinol
Phenyl methyl carbinol
Styralyl alcohol
1-Phenyl ethanol

Molecular Formula: $C_8H_{10}O$

Structure:



Chemical Properties

Molecular Weight: 122.16

Vapor Pressure: 0.25 mm at 25°C

Boiling Point: 203°C at 760 mm

Density: 1.0129 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.21

Melting Point: 20.7°C

Solubility: Slightly soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	400 mg/kg	rat	oral
	2500 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl bromide

CHEMICAL NAME

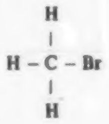
CAS Number: 74-83-9

Chemical Name: Bromomethane

Synonyms: Methyl bromide

Molecular Formula: CH_3Br

Structure:



$$\begin{array}{c} H \\ | \\ H-C-Br \\ | \\ H \end{array}$$

Chemical Properties

Molecular Weight: 94.95

Vapor Pressure: 1370 mm at 25°C

Boiling Point: 3.56°C at 760 mm

Density: 1.6755 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Volatile liquid or gas

Vapor Density: 3.72

Melting Point: -93.6°C

Solubility: Slightly (13.4 gm/l) (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate
Explosion–moderate
Disaster hazard–dangerous–toxic fumes–bromides

Methyl bromide

PRODUCTION DATA

Annual U.S. Production: 24.6 x 10^6 lbs. (1972)

Consumption: 24.6 x 10^6 lbs.

Fraction of Dispersion: 0.90

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 22.4

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LC_{50}	21 mg/l	rat	inhalation
LC_{Lo}	514 ppm (6 hours)	rat	inhalation
	6425 ppm (1 hour)	rabbit	inhalation
	300 ppm (9 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Irritate of eyes, skin, and mucous membranes

Damage to liver and kidney

CNS effects			
TC_{Lo}	35 ppm	human	inhalation
Skin effects			
TC_{Lo}	8000 ppm	human	skin

Chronic Toxicity

U.S. Occupational Standard: (air) Ceiling 20 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 20 ppm

Other Chronic Effects:

Nausea, vomiting, headache after ~ 35 ppm for two weeks

Severe lung iritation

Methyl butyl ketone

CHEMICAL NAME

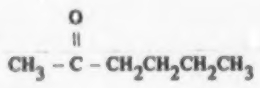
CAS Number: 591-78-6

Chemical Name: Methyl n-butyl ketone

Synonyms: 2-Hexanone
n-Butyl methyl ketone

Molecular Formula: $C_6H_{12}O$

Structure:



$CH_3 - \overset{\overset{O}{\|}}{C} - CH_2CH_2CH_2CH_3$

Chemical Properties

Molecular Weight: 100.16

Vapor Pressure: 10 mm at 38.8°C

Boiling Point: 128°C at 760 mm

Density: 0.81127 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.38

Physical State: Liquid

Vapor Density: 3.45

Melting Point: -57°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–moderate

Methyl butyl ketone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2590 mg/kg	rat	oral
LD_{Lo}	914 mg/kg	rat	intraperitoneal
	914 mg/kg	guinea pig	oral
LC_{Lo}	6000 ppm (7 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Irritant to eyes and respiratory tract

CNS depressant

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylbutynol

CHEMICAL NAME

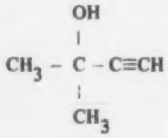
CAS Number: 115-19-5

Chemical Name: 2-Methyl-3-butyn-2-ol

Synonyms: Methyl butynol
1,1-Dimethyl-2-propynol
Ethynyldimethylcarbinol

Molecular Formula: C_5H_8O

Structure:



$$CH_3-\underset{CH_3}{\overset{OH}{C}}-C\equiv CH$$

Chemical Properties

Molecular Weight: 84.13

Vapor Pressure:

Boiling Point: 104°C at 760 mm

Density: 0.8618 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: 3.0°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–moderate

Methylbutynol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3600 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl cellulose

CHEMICAL NAME

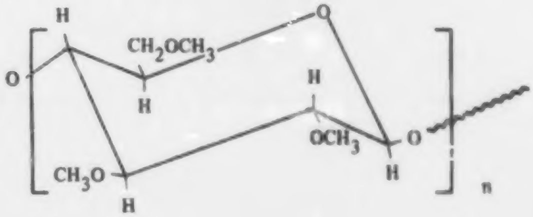
CAS Number: 9004-67-5

Chemical Name: Methyl ether cellulose

Synonyms:
Methyl cellulose
Cellulose methyl ether
Methocel

Molecular Formula: $[C_9H_{16}O_5]_n$

Structure:



Chemical Properties

Molecular Weight: 40,000-180,000

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methyl cellulose

PRODUCTION DATA

Annual U.S. Production: 20×10^6 lbs.

Consumption: 13×10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 13.6

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl chloride

CHEMICAL NAME

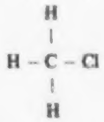
CAS Number: 74-87-3

Chemical Name: Chloromethane

Synonyms: Methyl chloride

Molecular Formula: CH_3Cl

Structure:



$$\mathrm{H}-\overset{\mathrm{H}}{\underset{\mathrm{H}}{\mathrm{C}}}-\mathrm{Cl}$$

Chemical Properties

Molecular Weight: 50.49

Vapor Pressure: 2.83 atm at 25°C

Boiling Point: -24.2°C at 760 mm

Density: 0.9159 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Gas

Vapor Density: 1.78

Melting Point: -97.73°C

Solubility: Soluble (4.9 gm/l H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts with oxidizing materials
Reacts slowly with RO_2 and O_3
$t_{1/2}$ with OH = 1 year

Safety Hazard: Fire–dangerous
Explosion–moderate
Disaster hazard–dangerous–toxic fumes–chlorides

Methyl chloride

PRODUCTION DATA

Annual U.S. Production: 458×10^6 lbs. (1974)

Consumption: 312×10^6 lbs. (1975)

Fraction of Dispersion: 0.03

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 18.1

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1800 mg/kg	rat	oral
LC_{Lo}	3000 ppm (4 hours)	rat	inhalation
	3146 ppm (7 hours)	mouse	inhalation
	20,000 ppm (2 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

- Slight irritant
- Narcotic
- CNS damage
- Damage to bone, liver, kidney, and cardiovascular system
- Pulmonary edema
- Conjunctivitis
- Anemia

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm
Ceiling 200 ppm
Peak 300 ppm/5 min/3 hours

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Methylcholanthrene

CHEMICAL NAME

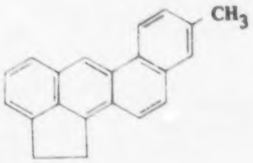
CAS Number: 56-49-5

Chemical Name: 3-Methyl cholanthrene

Synonyms: 20-Methylcholanthrene
1,2-Dihydro-3-methylbenz(j) aceanthrylene

Molecular Formula: $C_{21}H_{16}$

Structure:



Chemical Properties

Molecular Weight: 268.3

Vapor Pressure:

Boiling Point: 280°C at 80 mm

Density: 1.28 at 20°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methylcholanthrene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	100 mg/kg	mouse	intraperitoneal
	11 mg/kg	frog	intrarenal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	280 mg/kg	rat	oral
	18 mg/kg	rat	subcutaneous
	3 mg/kg	rat	parenteral
	100 mg/kg (5 weeks)	rat	intratracheal
	800 μg/kg	rat	implant
	13 mg/kg (42 weeks)	mouse	skin
	312 μg/kg	mouse	subcutaneous
	120 mg/kg	mouse	intratracheal
	132 mg/kg (12 weeks)	rabbit	intratracheal
	4 mg/kg	guinea pig	intraperitoneal
	40 mg/kg (15 days)	guinea pig	subcutaneous
	58 mg/kg	hamster	implant
	4500 mg/kg (8 weeks)	chicken	intraperitoneal
	27 mg/kg	duck	intratracheal
Neoplasm TD_{Lo}	34 mg/kg (25 weeks)	rat	skin
	39 mg/kg (6 days)	rat	intravenous
	1600 mg/kg (20 weeks)	mouse	intraperitoneal
	40 mg/kg	dog	implant
	100 mg/kg (9 weeks)	rabbit	implant
	3320 mg/kg (40 weeks)	hamster	skin

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylcyclohexane

CHEMICAL NAME

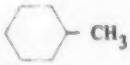
CAS Number: 108-87-2

Chemical Name: Methylcyclohexane

Synonyms: Hexahydrotoluene
Cyclohexylmethane

Molecular Formula: C_7H_{14}

Structure:



Chemical Properties

Molecular Weight: 98.19

Vapor Pressure: 47.06 mm at 25°C

Boiling Point: 100.9°C at 760 mm

Density: 0.7694 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.39

Melting Point: -126.59°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Fire–dangerous
Explosion–moderate

Methylcyclohexane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	4000 mg/kg	rabbit	oral
LC_{50}	7500 ppm (70 minutes)	rabbit	inhalation

Non-lethal Acute Effects:

Irritates skin

Narcosis and anesthesia

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 500 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 500 ppm

Other Chronic Effects:

Methylcyclohexanol

CHEMICAL NAME

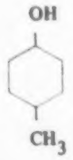
CAS Number: 25639-42-3

Chemical Name: Methylcyclohexanol

Synonyms:
4-Methyl cyclohexanol
Hexahydromethyl phenol
Hexahydro cresol

Molecular Formula: $C_7H_{14}O$

Structure:



Chemical Properties

Molecular Weight: 114.19

Vapor Pressure: <10 mm at 25°C

Boiling Point: 173 to 174°C at 760 mm

Density: 0.9170 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.93

Melting Point: -9.2°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Disaster hazard–dangerous–toxic fumes

Methylcyclohexanol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	1750 mg/kg	rabbit	oral

Non-lethal Acute Effects:

Irritant to eyes and trachea
Leucopenia

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Methylcyclohexanone

CHEMICAL NAME

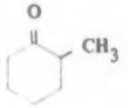
CAS Number: 583-60-8

Chemical Name: 2-Methyl cyclohexanone

Synonyms:

Molecular Formula: $C_7H_{12}O$

Structure:



Chemical Properties

Molecular Weight: 112.17

Vapor Pressure: <5 mm at 25°C

Boiling Point: 165°C at 757 mm

Density: 0.9250 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.86

Melting Point: -13.9°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Methylcyclohexanone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2140 mg/kg	rat	oral
LD_{Lo}	1000 mg/kg	rabbit	oral

Non-lethal Acute Effects:

Local irritant
Damage to liver and kidney

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

4, 4'-Methylenebis(2-chloroaniline)

CHEMICAL NAME

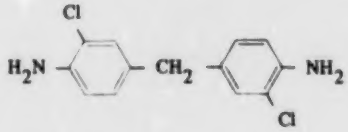
CAS Number: 101-14-4

Chemical Name: 4,4'-Methylenebis[2-chloro benzenamine]

Synonyms:
4,4'-Methylene-bis(2 chloroaniline)
Bisamine
Diamino-3-chlorophenyl-methane
Cyanaset
Dacpm
Curalin

Molecular Formula: $C_{13}H_{12}Cl_2N_2$

Structure:



Chemical Properties

Molecular Weight: 267.16

Vapor Pressure: Negligible

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 104 to 107°C

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

4, 4'-Methylenebis(2-chloroaniline)

PRODUCTION DATA

Annual U.S. Production: 7.716 x 10^6 lbs. (1972)

Consumption:

Fraction of Dispersion: 0.01

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 0.1

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:			
TD_{Lo}	420 gm/kg (80 weeks)	rat	oral
	2500 mg/kg (88 weeks)	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylene chloride

CHEMICAL NAME

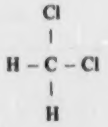
CAS Number: 75-09-2

Chemical Name: Dichloromethane

Synonyms: Methylene chloride
Methylene dichloride

Molecular Formula: CH_2Cl_2

Structure:



$$\begin{array}{c} Cl \\ | \\ H - C - Cl \\ | \\ H \end{array}$$

Chemical Properties

Molecular Weight: 84.93

Vapor Pressure: 435.8 mm at 25°C

Boiling Point: 40°C at 760 mm

Density: 1.3266 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.93

Melting Point: -95.1°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD: Total theoretical oxygen demand–0.38 gm/gm

Atmospheric Reactivity:
Not very active towards O_3 and RO_3
$t_{1/2}$ = 1 year with OH

Safety Hazard: Explosion–minor
Disaster hazard–dangerous–toxic fumes–phosgene

Methylene chloride

PRODUCTION DATA

Annual U.S. Production: 591 x 10^6 lbs. (1974)

Consumption: Estimated as 110 to 120 x 10^6 lbs. (1975)

Fraction of Dispersion: 0.95

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 366.8

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2136 mg/kg	rat	oral
	1500 mg/kg	mouse	intraperitoneal
	6460 mg/kg	mouse	subcutaneous
LD_{100}	950 mg/kg	dog	intraperitoneal
	1900 mg/kg	rabbit	oral
LD_{Lo}	3000 mg/kg	dog	oral
	2700 mg/kg	dog	subcutaneous
	200 mg/kg	dog	intravenous
	2700 mg/kg	rabbit	subcutaneous
	5000 ppm (2 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Central nervous system effects: narcosis

TC_{Lo} 500 ppm (1 year) intermittent

Blood effects:

TC_{Lo} 500 ppm (8 hours)

Chronic Toxicity

U.S. Occupational Standard: (air)
TWA 500 ppm
Ceiling 1000 ppm
Peak 2000 ppm/5 minutes/2 hours

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 500 ppm

Other Chronic Effects:
- Dermatitis
- Liver damage
- Reduced growth size

Methylenedianiline

CHEMICAL NAME

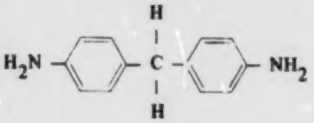
CAS Number: 101-77-9

Chemical Name: 4,4′-Methylenedianiline

Synonyms: Methylenedianiline

Molecular Formula: $C_{13}H_{14}N_2$

Structure:



Chemical Properties

Molecular Weight: 198.3

Vapor Pressure: <10 mm at 25°C

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 90°C

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard: Disaster hazard—dangerous—toxic fumes—aniline

Methylenedianiline

PRODUCTION DATA

Annual U.S. Production: 2.205 x 10^6 lbs.

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	347 mg/kg	rat	oral
	280 mg/kg	rat	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Carcinogen:			
TD_{Lo}	80 mg/kg	rat	oral
Neoplasm:			
TD_{Lo}	1410 mg/kg	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyldioxolane

CHEMICAL NAME

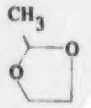
CAS Number: 1331-09-5

Chemical Name: Methyl dioxolane

Synonyms: 2-Methyl-3-dioxolane

Molecular Formula: $C_4H_8O_2$

Structure:



Chemical Properties

Molecular Weight: 88.12

Vapor Pressure:

Boiling Point: 81 to 82°C at 760 mm

Density: 0.9811 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.03

Melting Point:

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methyl dioxolane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl ethyl ketone

CHEMICAL NAME

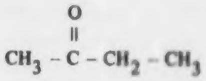
CAS Number: 78-93-3

Chemical Name: 2-Butanone

Synonyms: Methyl ethyl ketone
Methyl acetone

Molecular Formula: C_4H_8O

Structure:



$CH_3-\overset{O}{\overset{\|}{C}}-CH_2-CH_3$

Chemical Properties

Molecular Weight: 72.12

Vapor Pressure: 96.4 mm at 25°C

Boiling Point: 79.6°C at 760 mm

Density: 0.8054 at 20°C/4°C

Octanol/Water Partition Coefficient: 0.29

Physical State: Liquid

Vapor Density: 2.41

Melting Point: -86.35°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD: 89% of theoretical after 20 days at 20°C
Total theoretical oxygen demand 2.44 gm/gm

Atmospheric Reactivity:
Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate

Methyl ethyl ketone

PRODUCTION DATA

Annual U.S. Production: 509 x 10^6 lbs.

Consumption: 544.3 x 10^6 lbs.

Fraction of Dispersion: 0.95

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 524.7

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3400 mg/kg	rat	oral
	616 mg/kg	mouse	intraperitoneal
LD_{Lo}	2000 mg/kg	rat	intraperitoneal
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Non-lethal Acute Effects:

Local irritation and narcosis

Numbness of fingers and arms: 300 to 600 ppm

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

Other Chronic Effects:

Local irritation and narcosis

TLV: 200 ppm

Odor perception: 25 ppm

Methyl formate

CHEMICAL NAME

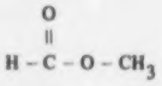
CAS Number: 107-31-3

Chemical Name: Formic acid, methyl ester

Synonyms: Methyl methanoate
Methyl formate

Molecular Formula: $C_2H_4O_2$

Structure:



$$H-\overset{\overset{\displaystyle O}{\|}}{C}-O-CH_3$$

Chemical Properties

Molecular Weight: 60.05

Vapor Pressure: 602.5 mm at 25°C

Boiling Point: 32.0°C

Density: 0.975 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 2.07

Melting Point: -99°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Explosion–moderate
Disaster hazard–dangerous–toxic fumes

Methyl formate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1620 mg/kg	rabbit	oral
LD_{Lo}	10,000 ppm	guinea pig	inhalation

Non-lethal Acute Effects:
Irritation of conjunctivia and optic nerve

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Methylhydrazine

CHEMICAL NAME

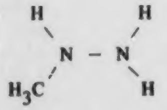
CAS Number: 60-34-4

Chemical Name: Methylhydrazine

Synonyms: Monomethyl hydrazine

Molecular Formula: CH_6N

Structure:



Chemical Properties

Molecular Weight: 46.07

Vapor Pressure: 49.6 mm at 25°C

Boiling Point: 87°C at 745 mm

Density: 0.874 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 1.6

Melting Point: <-80°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methylhydrazine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	183 mg/kg	rat	skin
	21 mg/kg	rat	intraperitoneal
	17 mg/kg	rat	intravenous
	33 mg/kg	rat	oral
	33 mg/kg	mouse	oral
	96 mg/kg	rabbit	skin
	12 mg/kg	rabbit	intravenous
	49 mg/kg	guinea pig	skin
	22 mg/kg	hamster	oral
	239 mg/kg	hamster	skin
	21 mg/kg	hamster	intraperitoneal
LC_{50}	74 ppm (4 hours)	rat	inhalation
	56 ppm (4 hours)	mouse	inhalation
	96 ppm (1 hour)	dog	inhalation
	82 ppm (1 hour)	monkey	inhalation
	143 ppm (4 hours)	hamster	skin

Chronic Toxicity

U.S. Occupational Standard: (air) 0.2 ppm
Ceiling 350 $\mu g/m^3$ (skin)

Carcinogenicity:

	3000 mg/kg (47 weeks)	hamster	oral

Mutagenicity:

Teratogenicity:

TLV:

TD_{Lo}	100 mg/kg (8-12 days)	mouse	oral
	200 mg/kg (14 days)	rabbit	oral

Other Chronic Effects:

Methyl iodide

CHEMICAL NAME

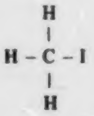
CAS Number: 74-88-4

Chemical Name: Iodomethane

Synonyms: Methyliodide

Molecular Formula: CH_3I

Structure:



$$\begin{array}{c} H \\ | \\ H - C - I \\ | \\ H \end{array}$$

Chemical Properties

Molecular Weight: 141.94

Vapor Pressure: 400 mm at 25.3°C

Boiling Point: 42.4°C at 760 mm

Density: 2.279 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.80

Physical State: Liquid

Vapor Density: 4.89

Melting Point: -66.45°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Residence in atmosphere: 0.003 year

Safety Hazard: Disaster hazard–dangerous–toxic fumes–iodides

Methyl iodide

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD$_{50}$	220 mg/kg	rat	oral
	110 mg/kg	mouse	subcutaneous
LD$_{Lo}$	800 mg/kg	rat	skin
LC$_{Lo}$	426 mg/m^3 (24 hours)	mouse	inhalation

Non-lethal Acute Effects:

Strong narcotic and anaesthetic
Irritant
Nausea and vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm (skin)

Carcinogenicity:

Neoplasm TD$_{Lo}$	50 mg/kg	rat	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl isoamyl ketone

CHEMICAL NAME

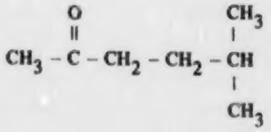
CAS Number: 110-12-3

Chemical Name: 5-Methyl-2-hexanone

Synonyms: Methyl iso-amyl ketone
MIAR

Molecular Formula: $C_7H_{14}O$

Structure:



$CH_3-\overset{\overset{O}{\|}}{C}-CH_2-CH_2-\underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{CH}}$

Chemical Properties

Molecular Weight: 114.19

Vapor Pressure:

Boiling Point: 144°C at 760 mm

Density: 0.888 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methyl isoamyl ketone

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4760 mg/kg	rat	oral
LD_{Lo}	3200 mg/kg	mouse	oral
LC_{Lo}	2000 ppm (4 hours)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl isobutyl ketone

CHEMICAL NAME

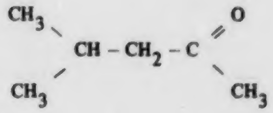
CAS Number: 108-10-1

Chemical Name: 4-Methyl-2-pentanone

Synonyms:
Methyl isobutyl ketone
Isobutyl methyl ketone
Hexone
Isopropylacetone
MIBK

Molecular Formula: $C_6H_{12}O$

Structure:



Chemical Properties

Molecular Weight: 100.16

Physical State: Liquid

Vapor Pressure: 7.1 mm at 25°C

Vapor Density: 3.45

Boiling Point: 116.85°C at 760 mm

Melting Point: −84.7°C

Density: 0.7978 at 20°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD: 69% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 2.7·gm/gm

Atmospheric Reactivity:
Reacts vigorously with reducing materials

Safety Hazard: Fire–moderate

Methyl isobutyl ketone

PRODUCTION DATA

Annual U.S. Production: 208.3×10^6 lbs.

Consumption: 208.3×10^6 lbs.

Fraction of Dispersion: 0.95

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 201.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	268 mg/kg	mouse	intraperitoneal
	2080 mg/kg	rat	oral
LD_{Lo}	2850 mg/kg	mouse	oral
LC_{Lo}	4000 ppm (15 minutes)	rat	inhalation

Non-lethal Acute Effects:

Irritation effects			
TC_{Lo}	200 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

Other Chronic Effects:

TLV: 100 ppm
Odor perception: 8 ppm

Methyl isocyanate

CHEMICAL NAME

CAS Number: 624-83-9

Chemical Name: Isocyanic acid, methyl ester

Synonyms: Methyl isocyanate
Methyl carbylamine

Molecular Formula: C_2H_3NO

Structure: $CH_3-N=C=O$

Chemical Properties

Molecular Weight: 57.05

Vapor Pressure:

Boiling Point: 59.6°C

Density: 0.9230 at 27°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -45°C

Solubility: Soluble (H_2O)
Reacts with H_2O

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methyl isocyanate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LC_{50}	14 ppm (4 hours)	rat	inhalation
	10 ppm (4 hours)	mouse	inhalation
	8 ppm (4 hours)	rabbit	inhalation
	13 ppm (4 hours)	guinea pig	inhalation
Non-lethal Acute Effects:			
Pulmonary edema			
TC_{Lo}	0.5 ppm	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 0.02 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl mercaptan

CHEMICAL NAME

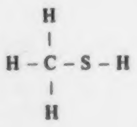
CAS Number: 74-93-1

Chemical Name: Methanethiol

Synonyms: Methyl mercaptan

Molecular Formula: CH_4S

Structure:



$$\begin{array}{ccccccc} & & H & & & & \\ & & | & & & & \\ H & - & C & - & S & - & H \\ & & | & & & & \\ & & H & & & & \end{array}$$

Chemical Properties

Molecular Weight: 48.11

Vapor Pressure: 760 mm at 6.8°C

Boiling Point: 6.2°C

Density: 0.8665 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid or gas

Vapor Density: 1.66

Melting Point: -123°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–dangerous
Disaster hazard–dangerous–toxic fumes–SO_x

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2.4 mg/kg	mouse	subcutaneous
LC_{Lo}	10,000 ppm	rat	inhalation

Non-lethal Acute Effects:
Irritant

Chronic Toxicity

U.S. Occupational Standard: (air) Ceiling 10 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:** 0.5 ppm

Other Chronic Effects:

Methyl methacrylate

CHEMICAL NAME

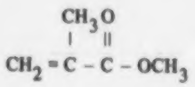
CAS Number: 80-62-6

Chemical Name: Methacrylic acid, methyl ester

Synonyms: Methyl methacrylate
2-Methyl propenoic acid, methyl ester

Molecular Formula: $C_5H_8O_2$

Structure:



$$CH_2=\overset{CH_3}{\overset{|}{C}}-\overset{O}{\overset{\|}{C}}-OCH_3$$

Chemical Properties

Molecular Weight: 100.13

Vapor Pressure: 40 mm at 25.5°C

Boiling Point: 100 to 101°C at 760 mm

Density: 0.9440 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.45

Melting Point: -48°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Explosion–moderate

Methyl methacrylate

PRODUCTION DATA

Annual U.S. Production: 718.8×10^6 lbs. (1974)

Consumption: 625×10^6 lbs.

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	7500 mg/kg	rat	subcutaneous
	1000 mg/kg	mouse	intraperitoneal
	6300 mg/kg	mouse	subcutaneous
	4500 mg/kg	dog	subcutaneous
	6300 mg/kg	guinea pig	oral
	2000 mg/kg	guinea pig	intraperitoneal
	6300 mg/kg	guinea pig	subcutaneous
LD_{Lo}	1800 mg/kg	rat	intraperitoneal
	5000 mg/kg	dog	oral
	6550 mg/kg	rabbit	oral
LC_{50}	3750 ppm	rat	inhalation
Non-lethal Acute Effects:			
Irritant effect			
TC_{Lo}	125 ppm	human	inhalation
Central nervous system effects			
TC_{Lo}	150 mg/m^3	human	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Methylnaphthalene

CHEMICAL NAME

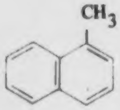
CAS Number: 1321-94-4

Chemical Name: Methylnaphthalene

Synonyms: 1-Methyl naphthalene

Molecular Formula: $C_{11}H_{10}$

Structure:



Chemical Properties

Molecular Weight: 142.21

Vapor Pressure: <10 mm at 25°C

Boiling Point: 244.64°C at 760 mm

Density: 1.0202 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point: -22°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Methylnaphthalene

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	5000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity: **TLV:**

Other Chronic Effects:

N-Methyl-N′-nitro-N-nitrosoguanidine

CHEMICAL NAME

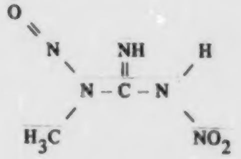
CAS Number: 70-25-7

Chemical Name: 1-Methyl-3-nitro-1-nitrosoguanidine

Synonyms: N-Methyl-N'-nitro-nitrosoguanidine
N'-Nitro-N-nitroso-N-methylguanidine

Molecular Formula: $C_2H_5N_5O_3$

Structure:



Chemical Properties

Molecular Weight: 147.1

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State:

Vapor Density:

Melting Point:

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

N-Methyl-N′-nitro-N-nitrosoguanidine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	400 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	75 mg/kg (4 weeks)	rat	oral
	40 mg/kg (4 weeks)	rat	intraperitoneal
	40 mg/kg (10 weeks)	rat	subcutaneous
	200 mg/kg (32 days)	rat	rectal
	100 mg/kg	mouse	oral
	200 mg/kg (22 weeks)	mouse	skin
	48 mg/kg	mouse	subcutaneous
	2457 mg/kg (66 weeks)	dog	oral
	740 mg/kg (27 weeks)	hamster	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methyl parathion

CHEMICAL NAME

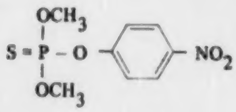
CAS Number: 298-00-0

Chemical Name: O,O-Dimethyl phosphorothioic acid O-(p-nitrophenyl) ester

Synonyms: Methyl parathion
O,O-Dimethyl-O-p-nitrophenyl phosphorothioate

Molecular Formula: $C_8H_{10}NO_5PS$

Structure:



Chemical Properties

Molecular Weight: 263.20

Vapor Pressure: 0.97 mm at 20°C

Boiling Point: Decomposes

Density: 1.358 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.44

Physical State: Solid

Vapor Density:

Melting Point: 35-36°C

Solubility: Slightly soluble (55 to 60 ppm H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Explosion–commercial product decomposes at 120°C with violence

Methyl parathion

PRODUCTION DATA

Annual U.S. Production: 51.1×10^6 lbs.

Consumption: 52.2×10^6 lbs.

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 52.7

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	9 mg/kg	rat	oral
	67 mg/kg	rat	skin
	3500 mg/kg	rat	intraperitoneal
	23 mg/kg	mouse	intraperitoneal
	9300 mg/kg	mouse	intraperitoneal
	30 mg/kg	mouse	subcutaneous
	300 mg/kg	rabbit	skin
	7 mg/kg	wild bird	oral
	25 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 200 $\mu g/m^3$

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylpentanediol

CHEMICAL NAME

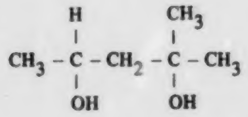
CAS Number: 107-41-5

Chemical Name: 2-Methyl-2,4-pentanediol

Synonyms: 2,4-Dihydroxy-2-methylpentane
α,α,α'-Trimethyltrimethylene glycol

Molecular Formula: $C_6H_{14}O_2$

Structure:



$$CH_3-\overset{\overset{\displaystyle H}{|}}{\underset{\underset{\displaystyle OH}{|}}{C}}-CH_2-\overset{\overset{\displaystyle CH_3}{|}}{\underset{\underset{\displaystyle OH}{|}}{C}}-CH_3$$

Chemical Properties

Molecular Weight: 118.06

Vapor Pressure: <0.1 mm at 20°C

Boiling Point: 198°C

Density:

Octanol/Water Partition Coefficient: -0.14

Physical State: Liquid

Vapor Density:

Melting Point: -50°C

Solubility: Infinite (H_2O)

Environmental Pursistence

BOD: 90% of theoretical after 20 days at 20°C
Total theoretical oxygen demand–2.3 (gm/gm)

Atmospheric Reactivity:

Safety Hazard:

Methylpentanediol

PRODUCTION DATA

Annual U.S. Production: 50 x 10^6 lbs.

Consumption: 50 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 50.8

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	3696 mg/kg	rat	oral
	3860 mg/kg	mouse	oral
	1299 mg/kg	mouse	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylpentynol

CHEMICAL NAME

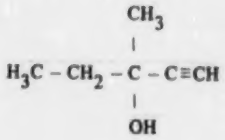
CAS Number: 77-75-8

Chemical Name: 3-Methyl-1-pentyn-3-ol

Synonyms: Methyl pentynol
2-Ethynyl-2-butanol
Dormison

Molecular Formula: $C_6H_{10}O$

Structure:



$$H_3C-CH_2-\overset{\overset{CH_3}{|}}{\underset{\underset{OH}{|}}{C}}-C\equiv CH$$

Chemical Properties

Molecular Weight: 98.15

Vapor Pressure:

Boiling Point: 120 to 121°C

Density: 0.8688 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.80

Physical State: Liquid

Vapor Density: 3.38

Melting Point: 30 to 31°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reactive toward oxidizing materials

Safety Hazard: Fire–slight

Methylpentynol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	300 mg/kg	rat	oral
	698 mg/kg	mouse	oral
	750 mg/kg	mouse	subcutaneous
	534 mg/kg	guinea pig	oral
Non-lethal Acute Effects:			
Psychotropic effects:			
TD_{Lo}	7 mg/kg	human	oral
Central nervous system effects:			
TD_{Lo}	70 mg/kg	human	oral
Dermatitis			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Methylphenylcarbinol

CHEMICAL NAME

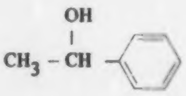
CAS Number: 98-85-1

Chemical Name: α-Methylbenzenemethanol

Synonyms:
Styralyl alcohol
Phenylmethylcarbinol
1-Phenethyl alcohol
1-Phenylethanol
α-Methylbenzyl alcohol

Molecular Formula: $C_8H_{10}O$

Structure:



Chemical Properties

Molecular Weight:	122.17	**Physical State:**	Liquid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:	204°C at 760 mm	**Melting Point:**	20.7°C
Density:	1.0135 at 20°C/4°C	**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

a-Methylstyrene

CHEMICAL NAME

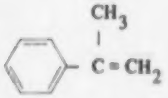
CAS Number: 1319-73-9

Chemical Name: Methyl styrene

Synonyms: α-Methyl styrene
Isopropenyl benzene
α-Phenyl propylene

Molecular Formula: C_9H_{10}

Structure:



Chemical Properties

Molecular Weight: 118.18

Vapor Pressure: 1 mm at 7.4°C

Boiling Point: 165.4°C at 760 mm

Density: 0.9106 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 4.08

Melting Point: -23.21°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:
Fire–moderate
Explosion–moderate

a-Methylstyrene

PRODUCTION DATA

Annual U.S. Production: 65×10^6 lbs. (1976 capacity)

Consumption: 50×10^6 lbs.

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	4900 mg/kg	rat	oral
LC_{Lo}	3000 ppm	rat	inhalation
	3000 ppm	guinea pig	inhalation

Non-lethal Acute Effects:

Irritant			
TC_{Lo}	600 ppm	human	inhalation
Conjunctivitis			
Dermatitis			

Chronic Toxicity

U.S. Occupational Standard: (air) TWA: 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Mevinphos

CHEMICAL NAME

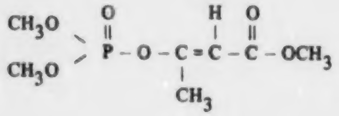
CAS Number: 298-01-1

Chemical Name: 3-[(Dimethoxyphosphinyl)oxy]-2-butenoic acid, methyl ester, (E)

Synonyms:
Mevinphos
2-Carbomethoxy-1-methyl-vinyldimethyl phosphate, α isomer
Phosdrin

Molecular Formula: $C_7H_{13}O_6P$

Structure:



$$\begin{matrix} CH_3O \\ CH_3O \end{matrix} > \overset{\overset{O}{\|}}{P}-O-\underset{\underset{CH_3}{|}}{C}=\overset{\overset{H}{|}}{C}-\overset{\overset{O}{\|}}{C}-OCH_3$$

Chemical Properties

Molecular Weight: 224.17

Vapor Pressure: 0.0029 at 21°C

Boiling Point: 99 to 103°C at 0.03 mm

Density: 1.25

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Infinite (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Mevinphos

PRODUCTION DATA

Annual U.S. Production: $<1 \times 10^6$ lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4 mg/kg	rat	oral
	4 mg/kg	rat	skin
	890 μg/kg	rat	intraperitoneal
	211 μg/kg	rat	subcutaneous
	4 mg/kg	mouse	oral
	3 mg/kg	mouse	intraperitoneal
	4700 μg/kg	rabbit	skin
	7520 μg/kg	chicken	oral
	3 mg/kg	wild bird	oral
LC_{50}	14 ppm (1 hour)	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 400 $\mu g/m^3$

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Mirex

CHEMICAL NAME

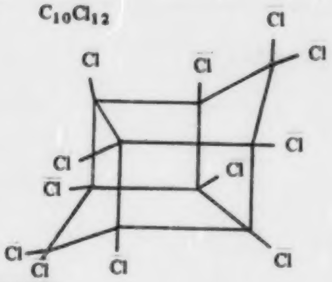
CAS Number: 2385-85-5

Chemical Name: 1,1a,2,2,3,3a,4,5,5,5a,5b,6-Dodecachlorooctahydro-1,3,4-metheno-l H-cyclobuta(cd) pentalene

Synonyms: Mirex
Dodecachloropentacyclo(3,3,2,$0^{2,6}$,$0^{3,9}$,$0^{7,10}$) decane

Molecular Formula: $C_{10}Cl_{12}$

Structure:



Chemical Properties

Molecular Weight: 545.6

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 485°C (decomposes,

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: $<1 \times 10^6$ lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	300-600 mg/kg	rat	oral
LD_{Lo}	306 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

TD_{Lo}	2222 mg/kg (58 weeks)	mouse	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Monosodium glutamate

CHEMICAL NAME

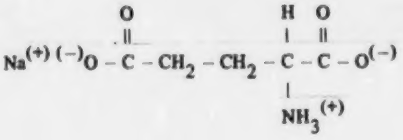
CAS Number: 142-47-2

Chemical Name: L – Glutamic acid, monosodium salt

Synonyms: Monosodium glutamate
MSG
Sodium-L-glutamate

Molecular Formula: $C_5H_9NO_4.N_a$

Structure:



$$\mathrm{Na}^{(+)}\,{}^{(-)}\mathrm{O}-\overset{\overset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{CH_2}-\mathrm{CH_2}-\underset{\underset{\mathrm{NH_3}^{(+)}}{|}}{\overset{\overset{\mathrm{H}}{|}}{\mathrm{C}}}-\overset{\overset{\mathrm{O}}{\|}}{\mathrm{C}}-\mathrm{O}^{(-)}$$

Chemical Properties

Molecular Weight: 170.14

Vapor Pressure: Negligible at 25°C

Boiling Point: Decomposes

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility: Soluble (739 gm/l H_2O)

Environmental Persistence

BOD: 65% of theoretical at 20°C for 5 days
Total theoretical oxygen demand = 1.42 gm/gm

Atmospheric Reactivity:

Safety Hazard:

Monosodium glutamate

PRODUCTION DATA

Annual U.S. Production: 47.3 x 10^6 lbs.

Consumption: 49.9 x 10^6

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 51.4

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	4253 mg/kg	rat	intraperitoneal
	8000 mg/kg	cat	subcutaneous
Non-lethal Acute Effects:			
Systematic effects:			
TD_{Lo}	43 mg/kg	human	oral
Chronic Toxicity			
U.S. Occupational Standard:			
Carcinogenicity:			
Mutagenicity:			
Teratogenicity:		TLV:	
TD_{Lo}	5 mg/kg	pregnant mouse (17 or 18 days)	parenteral
Other Chronic Effects:			

Morpholine

CHEMICAL NAME

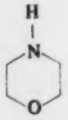
CAS Number: 110-91-8

Chemical Name: Morpholine

Synonyms: Tetrahydro-1,4- isoxazine
Diethethylenimide oxide

Molecular Formula: C_4H_9NO

Structure:



Chemical Properties

Molecular Weight: 87.12

Vapor Pressure: 10 mm at 23°C

Boiling Point: 128.3°C at 760 mm

Density: 1.0005 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.00

Melting Point: -4.75°C

Solubility: Infinite (H_2O)

Environmental Persistence

BOD: 0.9% of theoretical

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard: Fire–moderate
Disaster hazard–dangerous–toxic fumes–NO_x

Morpholine

PRODUCTION DATA

Annual U.S. Production: 23.3 x 10^6 lbs.

Consumption: 23.3 x 10^6 lbs.

Fraction of Dispersion: 0.50

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 12.4

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1050 mg/kg	rat	oral
	500 mg/kg	rabbit	skin

Non-lethal Acute Effects:

Local irritant

Kidney damage

Chronic Toxicity

U.S/ Occupational Standard: (air) TWA 20 ppm (skin)

Carcinogenicity:

Neoplastic effects: 6330 mg/kg (28 weeks) mouse oral

Mutagenicity:

Teratogenicity:

TLV: 20 ppm

Other Chronic Effects:

MSMA

CHEMICAL NAME

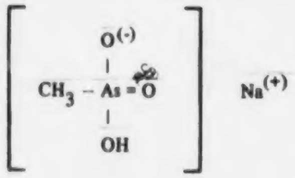
CAS Number: 2163-80-6

Chemical Name: Methanearsonic acid, monosodium salt

Synonyms: MSMA
Monosodium acid methane arsonate

Molecular Formula: $CH_4AsO_3 \cdot Na$

Structure:



$$\left[CH_3 - \overset{\overset{O^{(-)}}{|}}{\underset{\underset{OH}{|}}{As}} = O \right] Na^{(+)}$$

Chemical Properties

Molecular Weight: 162.97

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 161°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 35.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 35

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1800 mg/kg	rat	oral
	50 mg/kg	mammal	unreported

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Nabam

CHEMICAL NAME

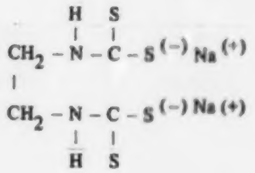
CAS Number: 142-59-6

Chemical Name: Ethylenebis(dithiocarbamic acid), disodium salt

Synonyms: Disodium ethylene bisdithiocarbamate

Molecular Formula: $C_4H_6N_2S_4 \cdot Na$

Structure:



$$\begin{array}{l} \phantom{CH_2 - {}} H \phantom{{} - {}} S \\ \phantom{CH_2 - {}} | \phantom{{} - {}} | \\ CH_2 - N - C - S^{(-)}\,Na^{(+)} \\ | \\ CH_2 - N - C - S^{(-)}\,Na^{(+)} \\ \phantom{CH_2 - {}} | \phantom{{} - {}} | \\ \phantom{CH_2 - {}} H \phantom{{} - {}} S \end{array}$$

Chemical Properties

Molecular Weight:	256.4	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	79 to 81°C
Density:		**Solubility:**	Soluble (H_2O)
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous, toxic fumes

Nabam

PRODUCTION DATA

Annual U.S. Production: 1.4 x 10^6 lbs. (1967)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	395 mg/kg	rat	oral
	580 mg/kg	mouse	oral

Non-lethal Acute Effects:

Irritant to skin and mucous membranes
Narcotic in high concentrations

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Potential carcinogen according to EPA

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Naled

CHEMICAL NAME

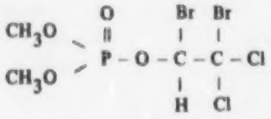
CAS Number: 300-76-5

Chemical Name: Phosphoric acid, 1,2-dibromo-2,2-dichloroethyl dimethyl ester

Synonyms: 1,2-Dibromo-2,2-dichloroethyl dimethylphosphate
Dimethyl-1,2-dibromo-2,2-dichloroethyl phosphate

Molecular Formula: $C_4H_7Br_2Cl_2O_4P$

Structure:



Chemical Properties

Molecular Weight: 380.7

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 270°C

Solubility: Insoluble (H_2O (hydrolyzes)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2.0

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	250 mg/kg	rat	oral
	800 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 3 mg/m^3

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Naphtha (solvent)

CHEMICAL NAME

CAS Number: MX 8030-31-7

Chemical Name: Coal tar naphtha

Synonyms: Solvent naphtha
Heavy naphtha
Hiflash naphtha

Molecular Formula:

Structure: (Mixture of xylene and higher homologs)

Chemical Properties

Molecular Weight:		**Physical State:**	Liquid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:	160 to 220°C	**Melting Point:**	
Density:	0.885 to 0.970	**Solubility:**	
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:
Reacts with oxidizing materials
Common air contaminant

Safety Hazard:
Fire–dangerous
Explosion–slight

Naphtha (solvent)

PRODUCTION DATA

Annual U.S. Production:	8288.4×10^6 lbs.	**Consumption:**	8288.4×10^6 lbs.
Fraction of Dispersion:	1.0	**Fraction of Production Lost:**	0.01

Release Rate (million lbs/yr): 8371.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	1600 ppm	rat	inhalation

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity: Recognized carcinogen

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Naphthalene

CHEMICAL NAME

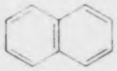
CAS Number: 91-20-3

Chemical Name: Naphthalene

Synonyms: Napthene

Molecular Formula: $C_{10}H_8$

Structure:



Chemical Properties

Molecular Weight: 128.19

Vapor Pressure: 0.2129 mm at 25°C

Boiling Point: 218°C

Density: 1.0253 at 20°C/4°C

Octanol/Water Partition Coefficient: 3.27

Physical State: Solid

Vapor Density: 4.42

Melting Point: 80.55°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD: Total theoretical oxygen demand: 3 gm/gm

Atmospheric Reactivity:

Reacts with oxidizing materials
Activity toward OH: $t_{1/2} = 2.5$ days
O_3: $t_{1/2} = 1$ year
RO_2: unreactive
Minor contaminant in air

Safety Hazard:

Fire–moderate
Explosion–moderate

Naphthalene

PRODUCTION DATA

Annual U.S. Production: 143 x 10^6 lbs. (1975)

Consumption: 140 x 10^6 lbs. (1975)

Fraction of Dispersion: 0.02

Fraction of Production Lost: 0.01

Release Rate (million lbs/yr): 16.9 (unspecified year)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1780 mg/kg	rat	oral
LD_{Lo}	100 mg/kg	child	oral
	150 mg/kg	mouse	intraperitoneal

Non-lethal Acute Effects:

Nausea
Anemia
Liver damage
Convulsions
Coma

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 10 ppm

Carcinogenicity:
Neoplasm
TD_{Lo} 3500 mg/kg (98 days intermittent)

Mutagenicity:

Teratogenicity:

TLV: 10 ppm

Other Chronic Effects:

a-Naphthalenesulfonic acid

CHEMICAL NAME

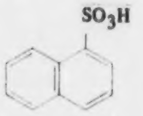
CAS Number: 85-47-2

Chemical Name: 1-Naphthalenesulfonic acid

Synonyms:

Molecular Formula: $C_{10}H_8O_3S$

Structure:



Chemical Properties

Molecular Weight: 208.25

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 139 to 140°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous, toxic fumes of SO_x

a-Naphthalenesulfonic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

B-Naphthalenesulfonic acid

CHEMICAL NAME

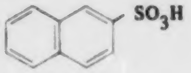
CAS Number: 120-18-3

Chemical Name: 2-Naphthalenesulfonic acid

Synonyms: Naphthaleno-2-sulfonic acid

Molecular Formula: $C_{10}H_8O_3S$

Structure:



Chemical Properties

Molecular Weight: 208.25

Vapor Pressure:

Boiling Point: Decomposes

Density: 1.441 at 25°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: 124 to 125°C

Solubility: Very soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous, toxic fumes of SO_x

B-Naphthalenesulfonic acid

PRODUCTION DATA

Annual U.S. Production: 39.0 x 10^6 lbs. (1968)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	400 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

a-Naphthol

CHEMICAL NAME

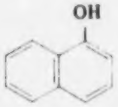
CAS Number: 90-15-3

Chemical Name: 1-Naphthol

Synonyms: 1-Hydroxynaphthalene

Molecular Formula: $C_{10}H_8O$

Structure:



Chemical Properties

Molecular Weight: 144.19

Vapor Pressure: 1 mm at 94°C

Boiling Point: 288°C (sublimes) at 760 mm

Density: 1.0989 at 99°C/4°C

Octanol/Water Partition Coefficient: 2.98

Physical State: Solid

Vapor Density:

Melting Point: 96°C

Solubility: Insoluble (H_2O)
Slightly soluble (hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

a-Naphthol

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2590 mg/kg	rat	oral
	880 mg/kg	rabbit	skin

Non-lethal Acute Effects:

- Nephritis
- Circulatory collapse
- Anemia
- Convulsions
- Injury to cornea and lens of eye

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

B-Naphthol

CHEMICAL NAME

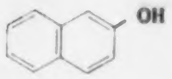
CAS Number: 135-19-3

Chemical Name: 2-Naphthol

Synonyms: 2-Hydroxynaphthalene
Naphthol B

Molecular Formula: $C_{10}H_8O$

Structure:



Chemical Properties

Molecular Weight: 144.19

Vapor Pressure: 15 mm at 128.6°C

Boiling Point: 295°C at 760 mm

Density: 1.28 at 20°C

Octanol/Water Partition Coefficient: 2.89

Physical State: Solid

Vapor Density: 4.97

Melting Point: 123 to 124°C

Solubility: Insoluble (H_2O)
Slightly soluble (hot H_2O)

Environmental Persistence

BOD: 93% of theoretical after 12 days

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

B-Naphthol

PRODUCTION DATA

Annual U.S. Production: (none in 1975 or 1976)

Consumption: 0.1×10^6 lbs. (1975)

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2420 mg/kg	rat	oral
LD_{Lo}	2940 mg/kg	rat	subcutaneous
	100 mg/kg	mouse	subcutaneous
	3800 mg/kg	rabbit	oral
	2670 mg/kg	guinea pig	subcutaneous

Non-lethal Effects:

- Nephritis
- Circulatory collapse
- Anemia
- Convulsions
- Damage to cornea and lens of eye

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1-Naphthylamine

CHEMICAL NAME

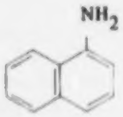
CAS Number: 134-32-7

Chemical Name: 1-Naphthylamine

Synonyms: α-Naphthylamine

Molecular Formula: $C_{10}H_9N$

Structure:



Chemical Properties

Molecular Weight: 143.20

Vapor Pressure: 1 mm at 104.3°C

Boiling Point: 300.8°C at 760 mm

Density: 1.1229 at 25°C/25°C

Octanol/Water Partition Coefficient: 2.22

Physical State: Solid

Vapor Density: 4.93

Melting Point: 50°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–slight–toxic fumes

1-Naphthylamine

PRODUCTION DATA

Annual U.S. Production: 1.1 x 10^6 lbs. (1963)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	779 mg/kg	rat	oral
LD_{Lo}	300 mg/kg	rabbit	subcutaneous
	4000 mg/kg	mammal	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Urinary bladder cancer			
TD_{Lo}	400 mg/kg	dog	subcutaneous
Neoplastic effects:			
TD_{Lo}	25 mg/kg	mouse	subcutaneous

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

2-Naphthylamine

CHEMICAL NAME

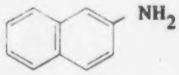
CAS Number: 91-59-8

Chemical Name: 2-Naphthylamine

Synonyms: β-Naphthylamine

Molecular Formula: $C_{10}H_9N$

Structure:



Chemical Properties

Molecular Weight: 143.20

Vapor Pressure: 1 mm at 108°C

Boiling Point: 306.1°C

Density: 1.0614 at 98°C/4°C

Octanol/Water Partition Coefficient: 2.25

Physical State: Solid

Vapor Density:

Melting Point: 113°C

Solubility: Soluble (H_2O)
(Very soluble in hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate–toxic fumes

2-Naphthylamine

PRODUCTION DATA

Annual U.S. Production: 1.28 x 10^6 lbs. (1955)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	727 mg/kg	rat	oral
	200 mg/kg	mouse	intraperitoneal
LD_{Lo}	500 mg/kg	dog	unknown

Chronic Toxicity

U.S. Occupational Standard: Carcinogen

Carcinogenicity:

TD_{Lo}	118 mg/kg (78 weeks)	rat	subcutaneous
	2120 mg/kg (52 weeks)	mouse	subcutaneous
	18 mg/kg	mouse	parenteral
	3900 mg/kg (2 years)	dog	oral
	14 mg/kg (240 weeks)	monkey	oral
	365 gm/kg (43 weeks)	hamster	oral
Neoplastic effects:			
TD_{Lo}	31 gm/kg (1 year)	rat	oral
	42 mg/kg	mouse	subcutaneous
	260 mg/kg (43 weeks)	hamster	oral

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Naptalam

CHEMICAL NAME

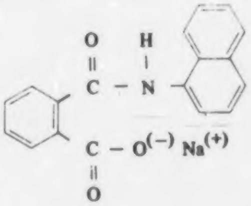
CAS Number: 132-67-2

Chemical Name: 2-[(1-Naphthalenylamino)carbonyl] benzoic acid, monosodium salt

Synonyms: N-Naphthyl phthalamic acid, sodium salt

Molecular Formula: $C_{18}H_{13}NO_3 \cdot Na$

Structure:



Chemical Properties

Molecular Weight:	291.3	**Physical State:**	Solid
Vapor Pressure:		**Vapor Density:**	
Boiling Point:		**Melting Point:**	185°C
Density:	1.40 at 20°C/4°C	**Solubility:**	0.2 gm/100 ml H_2O
Octanol/Water Partition Coefficient:			

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production: 2.0×10^6 lbs.

Consumption:

Fraction of Dispersion: Estimated as 1

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 2

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1770 mg/kg	rat	oral
	> 5 mg/kg	dog	oral

Non-lethal Acute Effects:
Relatively non-toxic to warm-blooded animals

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Neopentanoic acid

CHEMICAL NAME

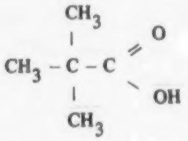
CAS Number: 75-98-9

Chemical Name: Pivalic acid

Synonyms: Neopentanoic acid
2,2-Dimethyl propanoic acid
Trimethyl acetic acid

Molecular Formula: $C_5H_{10}O_2$

Structure:



$$CH_3-\overset{\overset{CH_3}{|}}{\underset{\underset{CH_3}{|}}{C}}-C\genfrac{}{}{0pt}{}{\nearrow O}{\searrow OH}$$

Chemical Properties

Molecular Weight: 102.13

Vapor Pressure:

Boiling Point: 163.7 to 163.8°C at 760 mm

Density: 0.905 at 50°C

Octanol/Water Partition Coefficient: 1.60

Physical State: Solid

Vapor Density:

Melting Point: 35.3 to 35.5°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

PRODUCTION DATA

Annual U.S. Production: 5×10^6 lbs. (1975 capacity for neo-acids)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{Lo}	5000 mg/kg	rat	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Nitrilotriacetic acid, trisodium salt

CHEMICAL NAME

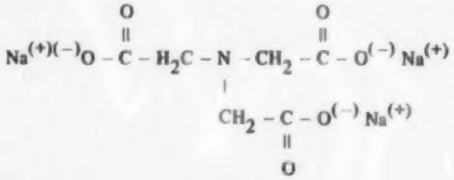
CAS Number: 5064-31-3

Chemical Name: N,N-bis(carboxymethyl)glycine, trisodium salt

Synonyms:
NTA, trisodium salt
Triglycine, trisodium salt
TGA, trisodium salt
Triglycolamic acid, trisodium salt

Molecular Formula: $C_6H_6NO_6 \cdot 3Na$

Structure:



$$\mathrm{Na^{(+)(-)}O-\overset{\overset{O}{\|}}{C}-H_2C-\underset{\underset{CH_2-\underset{\underset{O}{\|}}{C}-O^{(-)}\,Na^{(+)}}{|}}{N}-CH_2-\overset{\overset{O}{\|}}{C}-O^{(-)}\,Na^{(+)}}$$

Chemical Properties

Molecular Weight: 260.13

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point: Acid form -240°C with decomposition

Solubility: Soluble (H_2O)

Environmental Persistence

BOD: 76% of theoretical after 20 days at 20°C
Total theoretical oxygen demand = 0.93 gm/gm

Atmospheric Reactivity:

Safety Hazard:
Fire–combustible

Nitrilotriacetic acid, trisodium salt

PRODUCTION DATA

Annual U.S. Production: 85 x 10^6 lbs.

Consumption: 13 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr): 14.3

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1100 mg/kg	rat	oral
	254 mg/kg	rat	intraperitoneal
	681 mg/kg	mouse	oral
	750 mg/kg	monkey	oral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:
(Nitrilotriacetic acid is a confirmed carcinogen, causing urinary tract cancers in rats and mice.)

Mutagenicity:

Teratogenicity: Birth abnormalities may result from ingestion

TLV:

Other Chronic Effects:

p-Nitroaniline

CHEMICAL NAME

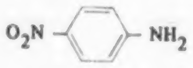
CAS Number: 100-01-6

Chemical Name: p-Nitroaniline

Synonyms: 1-Amino-4-nitrobenzene
Fast red 2G base

Molecular Formula: $C_6H_6N_2O_2$

Structure:



Chemical Properties

Molecular Weight: 138.13

Vapor Pressure: 1 mm at 142.4°C

Boiling Point: 331.73°C

Density: 1.424 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.41

Physical State: Solid

Vapor Density:

Melting Point: 148.5 to 149.5°C

Solubility: Insoluble (H_2O)
(Slightly in hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–slight

PRODUCTION DATA

Annual U.S. Production: 8.17×10^6 lbs. (1967)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	3249 mg/kg	rat	oral
	812 mg/kg	mouse	oral
	250 mg/kg	mouse	intraperitoneal
	75 mg/kg	wild bird	oral
LD_{Lo}	40 mg/kg	mammal	intravenous

Non-lethal Acute Effects:
Cyanosis
Nausea and vomiting
Convulsions

Chronic Toxicity

U.S. Occupational Standard: (air) 1 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 1 ppm (skin)

Other Chronic Effects:
Liver damage

Nitroanisole

CHEMICAL NAME

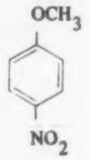
CAS Number: 100-17-4

Chemical Name: 1-Methoxy-4-nitrobenzene

Synonyms:

Molecular Formula: $C_7H_7NO_3$

Structure:



Chemical Properties

Molecular Weight: 153.14

Vapor Pressure:

Boiling Point: 276.8°C at 757 mm

Density: 1.2192 at 60°C/4°C

Octanol/Water Partition Coefficient: 2.03

Physical State: Solid

Vapor Density:

Melting Point: 54°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Nitroanisole

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD$_{50}$	4700 mg/kg	mammal (unspecified)	oral
	1400 mg/kg	mammal (unspecified)	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Nitrobenzene

CHEMICAL NAME

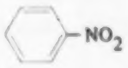
CAS Number: 98-95-3

Chemical Name: Nitrobenzene

Synonyms:
Oil of mirbane
Nitrobenzol
Mononitrobenzene
Artificial oil of bitter almonds
Solvent black 5
Nigrosine spirit soluble B

Molecular Formula: $C_6H_5NO_2$

Structure:



Chemical Properties

Molecular Weight: 123.06

Vapor Pressure: 0.284 mm at 25°C

Boiling Point: 210.8°C at 760 mm

Density: 1.2037 at 20°C/4°C

Octanol/Water Partition Coefficient: 1.88

Physical State: Solid/oily liquid

Vapor Density: 4.25

Melting Point: 5.7°C

Solubility: Slightly (1 gm/100 ml H_2O at 20°C)

Environmental Persistence

BOD: Total theoretical oxygen demand = 1.95 gm/gm

Atmospheric Reactivity:
Biodegradable
Unreactive to O_3 ($t_{1/2}$ = 11 years) and RO_2 ($t_{1/2}$ = 2000 years)
OH: $t_{1/2}$ = 3 days

Safety Hazard:
Fire–moderate
Explosion–moderate
Disaster hazard–moderate–toxic fumes–NO_x

Nitrobenzene

PRODUCTION DATA

Annual U.S. Production: 551.2×10^6 lbs. (1974)

Consumption: 551.2×10^6 lbs.

Fraction of Dispersion: 0.03

Fraction of Production Lost: 0.012

Release Rate (million lbs/yr): 19.3

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	800 mg/kg	rat	subcutaneous
	400 mg/kg	mouse	skin
	480 mg/kg	mouse	subcutaneous
	750 mg/kg	dog	oral
	150 mg/kg	dog	intravenous
	2000 mg/kg	cat	oral
	700 mg/kg	rabbit	oral
	600 mg/kg	rabbit	skin
	1000 mg/kg	mammal (unspecified)	oral
	ca. 80 mg/kg	human	oral

Non-lethal Acute Effects:

Blood effects			
TD_{Lo}	200 mg/kg	human female	oral

Cyanosis due to formation of methemoglobin

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 1 ppm (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity: 125 mg/kg subcutaneous **TLV:** 5 mg/m^3 (1 ppm)

In rat, caused delayed embryogenesis, embryo malformation and death

Other Chronic Effects:

Heart, liver and kidney damage

CNS effects

p-Nitrobenzoic acid

CHEMICAL NAME

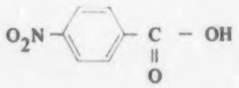
CAS Number: 62-23-7

Chemical Name: p-Nitrobenzoic acid

Synonyms: 4-Nitrobenzoic acid

Molecular Formula: $C_7H_5NO_4$

Structure:



Chemical Properties

Molecular Weight: 167.12

Physical State: Solid

Vapor Pressure: <10 mm at 25°C

Vapor Density:

Boiling Point: Sublimes

Melting Point: 242°C

Density: 1.610 at 20°C

Solubility: Insoluble (H_2O)

Octanol/Water Partition Coefficient: 2.03

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Diaster hazard–dangerous toxic fumes–NO_x

p-Nitrobenzoic acid

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD$_{50}$	1960 mg/kg	rat	oral
	1210 mg/kg	rat	intraperitoneal
	1960 mg/kg	rat	parenteral
	880 mg/kg	mouse	intraperitoneal
	770 mg/kg	mouse	intravenous
	1470 mg/kg	mouse	parenteral

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Nitrocellulose

CHEMICAL NAME

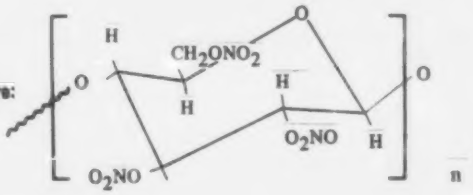
CAS Number: 9004-70-0

Chemical Name: Nitrate cellulose

Synonyms:
Nitrocellulose
Cellulose nitrate
Celloidin
Pyroxylin
Collodion

Molecular Formula: $(C_6H_7N_3O_{11})_n$

Structure:



$n = \geq 2$

Chemical Properties

Molecular Weight: $(297.13)_n$

Vapor Pressure: Negligible at 25°C

Boiling Point:

Density: 1.66

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–highly dangerous
Explosion–moderately dangerous

Nitrocellulose

PRODUCTION DATA

Annual U.S. Production: 50 x 10^6 lbs.

Consumption: 50 x 10^6 lbs.

Fraction of Dispersion: 1.0

Fraction of Production Lost: 0.03

Release Rate (million lbs/yr): 51.5

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
Low toxicity			

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Nitroethane

CHEMICAL NAME

CAS Number: 79-24-3

Chemical Name: Nitroethane

Synonyms:

Molecular Formula: $C_2H_5NO_2$

Structure: $CH_3 - CH_2 - NO_2$

Chemical Properties

Molecular Weight: 75.08

Vapor Pressure: 20.3 mm at 25°C

Boiling Point: 115°C at 760 mm

Density: 1.0448 at 25°C/4°C

Octanol/Water Partition Coefficient: 0.18

Physical State: Liquid

Vapor Density: 2.58

Melting Point: -50°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Fire–moderate
Explosion–dangerous
Disaster hazard–dangerous–toxic fumes NO_x

Nitroethane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1100 mg/kg	rat	oral
	860 mg/kg	mouse	oral
LD_{Lo}	500 mg/kg	rabbit	oral

Non-lethal Acute Effects:

Local irritant to eyes and respiratory tract

Dermatitis

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:

Nitroglycerine

CHEMICAL NAME

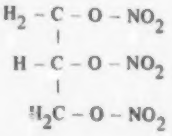
CAS Number: 55-63-0

Chemical Name: Nitroglycerine

Synonyms:
Ethylene glycol trinitrate
Glycerol trinitrate
Trinitrin
GNT
NT

Molecular Formula: $C_3H_5N_3O_9$

Structure:



$$\begin{array}{l} H_2 - C - O - NO_2 \\ \quad\;\; | \\ \;H - C - O - NO_2 \\ \quad\;\; | \\ \;\;H_2C - O - NO_2 \end{array}$$

Chemical Properties

Molecular Weight:	227.09	**Physical State:**	Liquid
Vapor Pressure:	1 mm at 127°C	**Vapor Density:**	7.84
Boiling Point:	256°C (explodes)	**Melting Point:**	13°C
Density:	1.5931 at 20°C/4°C	**Solubility:**	Slightly (H_2O)
Octanol/Water Partition Coefficient:	0.35		

Environmental Persistance

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–dangerous
Explosion–severe
Disaster hazard–very dangerous–toxic fumes

Nitroglycerine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	80 mg/kg	rat	oral
	40 mg/kg	rabbit	intravenous
	275 mg/kg	rat	intramuscular
	150 mg/kg	cat	subcutaneous
	400 mg/kg	rabbit	subcutaneous
	450 mg/kg	rabbit	intramuscular

Non-lethal Acute Effects:

- Respiratory paralysis
- Skin irritation
- Vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) 2 mg/m^3 (skin)

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 2 mg/m^3

Other Chronic Effects:

Nitromethane

CHEMICAL NAME

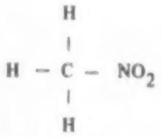
CAS Number: 75-52-5

Chemical Name: Nitromethane

Synonyms: Nitrocarbol

Molecular Formula: CH_3NO_2

Structure:



$$\begin{array}{c} \quad H \\ \quad | \\ H - C - NO_2 \\ \quad | \\ \quad H \end{array}$$

Chemical Properties

Molecular Weight: 61.04

Vapor Pressure: 36.27 mm at 25°C

Boiling Point: 100.8°C at 760 mm

Density: 1.1371 at 20°C/4°C

Octanol/Water Partition Coefficient: 0.17

Physical State: Liquid

Vapor Density: 2.11

Melting Point: -17°C

Solubility: Soluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity: Reacts with oxidizing materials

Safety Hazard:

Fire–dangerous
Explosion–moderate
Disaster hazard–dangerous–toxic fumes of NO_x

PRODUCTION DATA

Annual U.S. Production:	**Consumption:**
Fraction of Dispersion:	**Fraction of Production Lost:**

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	940 mg/kg	rat	oral
	950 mg/kg	mouse	oral
LD_{Lo}	125 mg/kg	dog	oral
	565 mg/kg	dog	subcutaneous
	800 mg/kg	dog	intravenous
	750 mg/kg	rabbit	oral
	750 mg/kg	rabbit	intravenous
LC_{Lo}	2446 mg/m^3	monkey	inhalation

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 100 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 100 ppm

Other Chronic Effects:
- Nausea
- Vomiting
- Kidney and liver damage
- Irritates eyes

m-Nitrophenol

CHEMICAL NAME

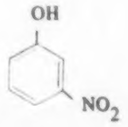
CAS Number: 554-84-7

Chemical Name: 3-Nitrophenol

Synonyms:

Molecular Formula: $C_6H_5NO_2$

Structure:



Chemical Properties

Molecular Weight: 139.11

Vapor Pressure: 10 mm at 25°C

Boiling Point: 194°C at 70 mm

Density: 1.2797 at 100°C/4°C

Octanol/Water Partition Coefficient: 2.05

Physical State: Solid

Vapor Density:

Melting Point: 97°C

Solubility: Slightly (H_2O)
(Very soluble in hot H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes–NO_x

m-Nitrophenol

PRODUCTION DATA

Annual U.S. Production: 14.8 x 10^6 lbs. (1967 all nitrophenols)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	447 mg/kg	rat	oral
	1414 mg/kg	mouse	oral
LD_{Lo}	83 mg/kg	dog	intravenous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Nitrophenol

CHEMICAL NAME

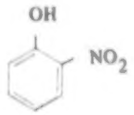
CAS Number: 88-75-5

Chemical Name: o-Nitrophenol

Synonyms: 2-Hydroxynitrobenzene

Molecular Formula: $C_6H_5NO_3$

Structure:



Chemical Properties

Molecular Weight: 139.11

Vapor Pressure: 1 mm at 49.3°

Boiling Point: 216°C at 760 mm

Density: 1.485 at 14°C

Octanol/Water Partition Coefficient: 3.58

Physical State: Solid

Vapor Density:

Melting Point: 45.3 to 45.7°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Diaster hazard—dangerous—toxic fumes NO_x

PRODUCTION DATA

Annual U.S. Production: 14.8 x 10^6 lbs. (1967 all nitrophenols)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2828 mg/kg	rat	oral
	1297 mg/kg	rat	oral
LD_{Lo}	100 mg/kg	dog	intravenous

Non-lethal Acute Effects:

Liver and kidney damage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

†TLV:

Other Chronic Effects:

p-Nitrophenol

CHEMICAL NAME

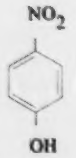
CAS Number: 100-02-7

Chemical Name: p-Nitrophenol
4-Nitrophenol

Synonyms:

Molecular Formula: $C_6H_5NO_3$

Structure:



Chemical Properties

Molecular Weight: 139.11

Physical State: Solid

Vapor Pressure:

Vapor Density:

Boiling Point: 279°C (decomposes)

Melting Point: 114.9 to 115.6°C

Density: 1.479 at 20°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 1.97

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes–NO_x

o-Nitrophenol

PRODUCTION DATA

Annual U.S. Production: 14.8×10^6 lbs. (1967 all nitrophenols)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	2828 mg/kg	rat	oral
	1297 mg/kg	rat	oral
LD_{Lo}	100 mg/kg	dog	intravenous

Non-lethal Acute Effects:
Liver and kidney damage

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Nitrophenol

PRODUCTION DATA

Annual U.S. Production: 52×10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.015

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	350 mg/kg	rat	oral
	467 mg/kg	mouse	oral
	75 mg/kg	mouse	intraperitoneal
	150 mg/kg	cat	intraperitoneal
LD_{Lo}	65 mg/kg	pigeon	intramuscular
	10 mg/kg	dog	intravenous
	500 mg/kg	dog	intraperitoneal

Non-lethal Acute Effects:
- Hyperthermia
- Methemoglobinemia
- CNS depression

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

1-Nitropropane

CHEMICAL NAME

CAS Number: 108-03-2

Chemical Name: 1-Nitropropane

Synonyms:

Molecular Formula: $C_3H_7NO_2$

Structure: $CH_3 - CH_2 - CH_2 - NO_2$

Chemical Properties

Molecular Weight: 81.11

Physical State: Liquid

Vapor Pressure: 9.87 mm at 25°C

Vapor Density: 3.06

Boiling Point: 130.5 to 131.5°C at 760 mm

Melting Point: -108°C

Density: 1.0081 at 24°C/4°C

Solubility: Slightly (H_2O)

Octanol/Water Partition Coefficient: 2.41

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate
Explosion–dangerous
Disaster hazard–dangerous–toxic fumes NO_x

1-Nitropropane

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	800 mg/kg	mouse	oral
LD_{Lo}	250 mg/kg	rabbit	oral
	1000 mg/kg	rat	oral

Non-lethal Acute Effects:

Irritation of eyes
Vomiting

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV: 25 ppm

Other Chronic Effects:

2-Nitropropane

CHEMICAL NAME

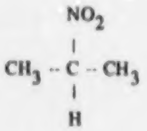
CAS Number: 79-46-9

Chemical Name: 2-Nitropropane

Synonyms: Isonitropropane

Molecular Formula: $C_3H_7NO_2$

Structure:



$$CH_3 - \overset{\displaystyle NO_2}{\overset{|}{\underset{\displaystyle H}{\underset{|}{C}}}} - CH_3$$

Chemical Properties

Molecular Weight: 89.09

Vapor Pressure: 17.42 mm at 25°C

Boiling Point: 120°C at 760 mm

Density: 0.9876 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 3.06

Melting Point: -93°C

Solubility: Slightly (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Fire–moderate
Explosion–dangerous
Disaster hazard–dangerous–toxic fumes–NO_x

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{Lo}	500 mg/kg	rat	oral
	75 mg/kg	mouse	intraperitoneal
	500 mg/kg	rabbit	oral
LC_{Lo}	1513 ppm (5 hours)	rat	inhalation
	714 ppm (5 hours)	cat	inhalation
	2381 ppm (5 hours)	rabbit	inhalation
	4622 ppm (5 hours)	guinea pig	inhalation

Non-lethal Acute Effects:

Central nervous system effects			
TD_{Lo}	15 ppm	human	inhalation
Local irritant			
Vomiting			

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 25 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity: TLV: 25 ppm

Other Chronic Effects:

N-Nitrosodiethylamine

CHEMICAL NAME

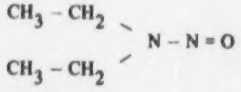
CAS Number: 55-18-5

Chemical Name: N-Nitrosodiethylamine

Synonyms:

Molecular Formula: $C_4H_{10}N_2O$

Structure:



Chemical Properties

Molecular Weight: 102.14

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 176.9°C at 760 mm

Melting Point:

Density: 0.9422 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

N-Nitrosodiethylamine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	216 mg/kg	rat	oral
	11 mg/kg	rat	intraperitoneal
	157 mg/kg	rat	intravenous
	246 mg/kg	hamster	unknown
Chronic Toxicity			
U.S. Occupational Standard:			
Carcinogenicity:			
TD_{Lo}	45 mg/kg (83 weeks)	rat	oral
	100 mg/kg	rat	intraperitoneal
	200 mg/kg (10-21 days pregnant)	rat	subcutaneous
	40 mg/kg	rat	intravenous
	57 mg/kg	mouse	oral
	560 mg/kg	dog	oral
	18 gm/kg	monkey	oral
	2 gm/kg	monkey	intraperitoneal
	960 mg/kg (28 weeks)	rabbit	oral
	750 mg/kg (2.2 years)	pig	oral
Mutagenicity:			
Teratogenicity:		TLV:	
TD_{Lo}	150 mg/kg (22 days pregnant)	rat	intravenous
	19 gm/kg (15-20 days pregnant)	mouse	unknown
	17 mg/kg (pregnant)	hamster	subcutaneous
Other Chronic Effects:			

N-Nitrosodimethylamine

CHEMICAL NAME

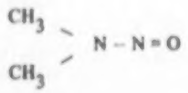
CAS Number: 62-75-9

Chemical Name: N-Nitrosodimethylamine

Synonyms: Dimethylnitrosamine
Nitrous dimethyl amide

Molecular Formula: $C_2H_6N_2O$

Structure:



Chemical Properties

Molecular Weight: 74.08

Physical State: Liquid

Vapor Pressure:

Vapor Density:

Boiling Point: 154°C at 760 mm

Melting Point:

Density: 1.0059 at 20°C/4°C

Solubility: Soluble (H_2O)

Octanol/Water Partition Coefficient:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Disaster hazard–dangerous–toxic fumes

N-Nitrosodimethylamine

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	26 mg/kg	rat	oral
	36 mg/kg	rat	intraperitoneal
	45 mg/kg	rat	subcutaneous
	40 mg/kg	rat	rectal
LC_{50}	78 ppm (4 hours)	rat	inhalation
	57 ppm (4 hours)	mouse	inhalation

Non-lethal Acute Effects:

- Irritant
- Gastrointestinal hemorrhage
- Liver damage

Chronic Toxicity

U.S. Occupational Standard: (air) Carcinogen

Carcinogenicity:			
TD_{Lo}	248 mg/kg (31 weeks)	rat	oral
	37 mg/kg	rat	inhalation
	30 mg/kg (35 weeks)	rat	rectal
	370 mg/kg (56 weeks)	mouse	oral
	4375 μg/kg	mouse	subcutaneous
	202 mg/kg (23 weeks)	rabbit	oral
Neoplastic effects:			
TD_{Lo}	30 mg/kg	rat	intraperitoneal
	18 mg/kg	rat	intramuscular
	18 mg/kg	rat	parenteral
	18 mg/kg	rat	intravenous
	7 mg/kg	mouse	intraperitoneal

Mutagenicity:

Teratogenicity:

TD_{Lo}	13 mg/kg	mouse	

TLV: unknown

Other Chronic Effects:

Nitrosoethylurea

CHEMICAL NAME

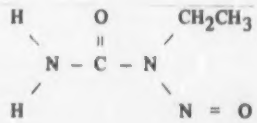
CAS Number: 759-73-9

Chemical Name: N-Ethyl-N-nitrosourea

Synonyms: 1-Ethyl,1-nitrosourea

Molecular Formula: $C_3H_7N_3O_2$

Structure:



Chemical Properties

Molecular Weight: 117.13

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient:

Physical State: Solid

Vapor Density:

Melting Point:

Solubility:

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

Nitrosoethylurea

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD$_{50}$	300 mg/kg	rat	oral
	240 mg/kg	rat	intravenous
Non-lethal Acute Effects:			
Dermatitis			
Chronic Toxicity			
U.S. Occupational Standard:			
Carcinogenicity:			
TD$_{Lo}$	10 mg/kg	rat	oral
	5 mg/kg	rat	subcutaneous
	20 mg/kg	rat	intravenous
	2200 mg/kg (9 weeks)	mouse	subcutaneous
Neoplasm TD$_{Lo}$	60 mg/kg	mouse	intraperitoneal
Mutagenicity:			
Teratogenicity:		**TLV:**	
TD$_{Lo}$	5 mg/kg (15 days pregnant)	rat	intravenous
	29 mg/kg (12-19 days pregnant)	mouse	intraperitoneal
	80 mg/kg (15 days pregnant)	rat	parenteral
	240 mg/kg (22-23 days pregnant)	pig	intravenous
Other Chronic Effects:			

Nitrosomethylurea

CHEMICAL NAME

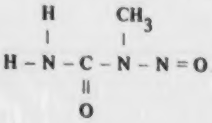
CAS Number: 684-93-5

Chemical Name: N-Methyl-N-nitrosourea

Synonyms: 1-Methyl,1-nitrosourea

Molecular Formula: $C_2H_5N_3O_2$

Structure:



$$\mathrm{H-\overset{\displaystyle H}{\overset{|}{N}}-\underset{\underset{\displaystyle O}{\|}}{C}-\overset{\displaystyle CH_3}{\overset{|}{N}}-N=O}$$

Chemical Properties

Molecular Weight: 103.08

Vapor Pressure:

Boiling Point:

Density:

Octanol/Water Partition Coefficient: -0.16

Physical State: Solid

Vapor Density:

Melting Point: 123 to 124°C (decomposes)

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

Nitrosomethylurea

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

	Dosage	Animal	Route
Acute Toxicity LD_{50}	180 mg/kg	rat	oral
	110 mg/kg	rat	intraperitoneal
	144 mg/kg	mouse	intraperitoneal
	115 mg/kg	hamster	subcutaneous

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:			
TD_{Lo}	230 mg/kg (24 weeks)	rat	intraperitoneal
	180 mg/kg (36 weeks)	rat	subcutaneous
	90 mg/kg	rat	oral
	202 mg/kg (30 weeks)	rat	skin
	70 mg/kg	rat	intravenous
	50 mg/kg	mouse	intraperitoneal
Mutagenicity:			
Teratogenicity:		**TLV:**	
TD_{Lo}	10 mg/kg (13 days)	rat	intraperitoneal
	12 mg/kg (15-23 days)	pregnant rat	intravenous

Other Chronic Effects:

m-Nitrotoluene

CHEMICAL NAME

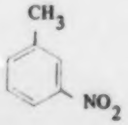
CAS Number: 99-08-1

Chemical Name: m-Nitrotoluene

Synonyms: 3-Methylnitrobenzene

Molecular Formula: $C_7H_7NO_2$

Structure:



Chemical Properties

Molecular Weight: 137.14
Vapor Pressure: 1 mm at 50°C
Boiling Point: 232.6°C at 760 mm
Density: 1.1571 at 20°C/4°C
Octanol/Water Partition Coefficient: 2.45

Physical State: Liquid
Vapor Density: 4.72
Melting Point: 16°C
Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	1072 mg/kg	rat	oral
	330 mg/kg	mouse	oral
	2400 mg/kg	rabbit	oral
	3600 mg/kg	guinea pig	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

o-Nitrotoluene

CHEMICAL NAME

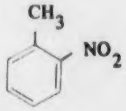
CAS Number: 88-72-7

Chemical Name: o-Nitrotoluene

Synonyms: 2-Methylnitrobenzene
2-Nitrotoluene

Molecular Formula: $C_7H_7NO_2$

Structure:



Chemical Properties

Molecular Weight: 137.14

Vapor Pressure: 1 mm at 50°C

Boiling Point: 220.4°C at 760 mm

Density: 1.1629 at 20°C

Octanol/Water Partition Coefficient: 2.30

Physical State: Liquid

Vapor Density: 4.72

Melting Point: -9.55°C

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–moderate

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	891 mg/kg	rat	oral
	2462 mg/kg	mouse	oral

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

p-Nitrotoluene

CHEMICAL NAME

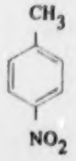
CAS Number: 99-99-0

Chemical Name: p-Nitrotoluene

Synonyms: 4-Methylnitrobenzene

Molecular Formula: $C_7H_7NO_2$

Structure:



Chemical Properties

Molecular Weight:	137.14	**Physical State:**	Solid
Vapor Pressure:	1 mm at 53.7°C	**Vapor Density:**	4.72
Boiling Point:	238.3°C at 760 mm	**Melting Point:**	54.5°C
Density:	1.1038 at 75°C/4°C	**Solubility:**	Insoluble (H_2O)
Octanol/Water Partition Coefficient:	2.42		

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:

p-Nitrotoluene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	**Dosage**	**Animal**	**Route**
LD_{50}	2144 mg/kg	rat	oral
	1231 mg/kg	mouse	oral
	940 mg/kg	mammal (unspecified)	intraperitoneal

Chronic Toxicity

U.S. Occupational Standard: (air) TWA 5 ppm

Carcinogenicity:

Mutagenicity:

Teratogenicity:

†TLV: 5 ppm (skin)

Other Chronic Effects:

Nonene

CHEMICAL NAME

CAS Number: 27215-95-8

Chemical Name: Nonene

Synonyms: Nonene (mixed isomers)
Nonylene

Molecular Formula: C_9H_{18}

Structure: $CH_3 - (CH_2)_6 - CH = CH_2$ (1 - Nonene)

Chemical Properties

Molecular Weight: 126.19

Vapor Pressure:

Boiling Point: 149.9°C (1-nonene)

Density: 0.7433 (1-nonene)

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density:

Melting Point:

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:

Safety Hazard:
Fire–combustible

Nonene

PRODUCTION DATA

Annual U.S. Production:

Consumption:

Fraction of Dispersion:

Fraction of Production Lost:

Release Rate (million lbs/yr):

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

Nonyl phenol

CHEMICAL NAME

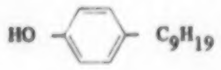
CAS Number: 25154-52-3

Chemical Name: Nonylphenol

Synonyms: p-Nonylphenol
Hydroxyl No. 253

Molecular Formula: $C_{15}H_{24}O$

Structure:



Chemical Properties

Molecular Weight: 220.34

Vapor Pressure: 10 mm at 25°C

Boiling Point: 290 to 302°C

Density: 0.949 at 20°C/4°C

Octanol/Water Partition Coefficient:

Physical State: Liquid

Vapor Density: 7.59

Melting Point:

Solubility: Insoluble (H_2O)

Environmental Persistence

BOD:

Atmospheric Reactivity:
Rapidly biodegraded
Not reactive to O_3 or RO_2
Reacts with oxidizing materials
$t_{1/2}$ OH = 2 days

Safety Hazard:
Fire–slight

Nonyl phenol

PRODUCTION DATA

Annual U.S. Production: 191 x 10^6 lbs. (1976 capacity)

Consumption:

Fraction of Dispersion:

Fraction of Production Lost: 0.007

Release Rate (million lbs/yr): 180.6 (ethoxylated compound)

TOXICITY DATA

Acute Toxicity	Dosage	Animal	Route
LD_{50}	1620 mg/kg	rat	oral
	2140 mg/kg	rabbit	skin

Chronic Toxicity

U.S. Occupational Standard:

Carcinogenicity:

Mutagenicity:

Teratogenicity:

TLV:

Other Chronic Effects:

BEST SELLERS NTIS

FROM NATIONAL TECHNICAL INFORMATION SERVICE

An Inexpensive Economical Solar Heating System for Homes
N76-27671/PAT 59 p PC$4.50/MF$3.00

Viking I: Early Results
N76-28296/PAT 76 p PC$2.00/MF$3.00

Energy Fact Book 1976, Chapters 1 through 21
ADA-028 284/PAT 432 p PC$11.75/MF$3.00

Security Analysis and Enhancements of Computer Operating Systems
PB-257 087/PAT 70 p PC$4.50/MF $3.00

Evaluation of the Air-to-Air Heat Pump for Residential Space Conditioning
PB-255 652/PAT 293 p PC$9.25/MF$3.00

Monitoring Groundwater Quality: Monitoring Methodology
PB-256 068/PAT 169 p PC$6.75/MF$3.00

An Air Force Guide to Software Documentation Requirements
ADA-027 051/PAT 178 p PC$7.50/MF$3.00

The Production of Oil from Intermountain West Tar Sands Deposits
PB-256 516/PAT 98 p PC$5.00/MF$3.00

Analysis of Large Scale Non-Coal Underground Mining Methods
PB-234 555/PAT 581 p PC$13.75/MF$3.00

Who's Who in the Interagency Energy/Environment R and D Program
PB-256 977/PAT 35 p PC$4.00/MF$3.00

Local Area Personal Income, 1969-1974. Volume 2: Central and Northeastern States
PB-254 056/PAT 578 p PC$13.75/MF$3.00

Feasibility of Considerably Expanded Use of Western Coal by Midwestern and Eastern Utilities in the Period 1978 and Beyond
PB-256 048/PAT 61 p PC$4.50/MF$3.00

Availability of Potential Coal Supply Through 1985 by Quality Characteristics
PB-256 680/PAT 121 p PC$5.50/MF$3.00

Flat-Plate Solar Collector Handbook: A Survey of Principles, Technical Data and Evaluation Results
UCID-17086/PAT 96 p PC$5.00/MF$3.00

HOW TO ORDER

When you indicate the method of payment, please note if a purchase order is not accompanied by payment, you will be billed an additional $5.00 *ship and bill* charge. And please include the card expiration date when using American Express.

Normal delivery time takes three to five weeks. It is vital that you order by number or your order will be manually filled, insuring a delay. You can opt for *airmail delivery* for $2.00 North American continent; $3.00 outside North American continent charge per item. Just check the *Airmail Service* box. If you're really pressed for time, call the NTIS Rush Handling Service (703) 557-4700. For a $10.00 charge per item, your order will be airmailed within 48 hours. Or, you can pick up your order in the Washington Information Center & Bookstore or at our Springfield Operations Center within 24 hours for a $6.00 per item charge.

You may also place your order by telephone or if you have an NTIS Deposit Account or an American Express card order through TELEX. The order desk number is (703) 557-4650 and the TELEX number is 89-9405.

Thank you for your interest in NTIS. We appreciate your order.

METHOD OF PAYMENT

☐ Charge my NTIS deposit account no. ____________
☐ Purchase order no. ____________
☐ Check enclosed for $ ____________
☐ Bill me. Add $5.00 per order and sign below. (Not available outside North American continent.)
☐ Charge to my American Express Card account number

☐☐☐☐☐☐☐☐☐☐☐☐☐☐☐

Card expiration date ____________
Signature ____________
☐ Airmail Services requested

NAME ____________
ADDRESS ____________
CITY, STATE, ZIP ____________

Item Number	Quantity		Unit Price*	Total Price**
	Paper Copy (PC)	Microfiche (MF)		
			Sub Total	
			Additional Charge	
			Enter Grand Total	

All prices subject to change. The prices above are accurate as of 3/77.

Foreign Prices on Request.

Clip and mail to:

NTIS
National Technical Information Service
U.S. DEPARTMENT OF COMMERCE
Springfield, Va. 22161
(703) 557-4650 TELEX 89-9405